

Supplementary Information for:

Using Genetic Algorithms to Discover Novel

High-Spin Conjugated Polymers

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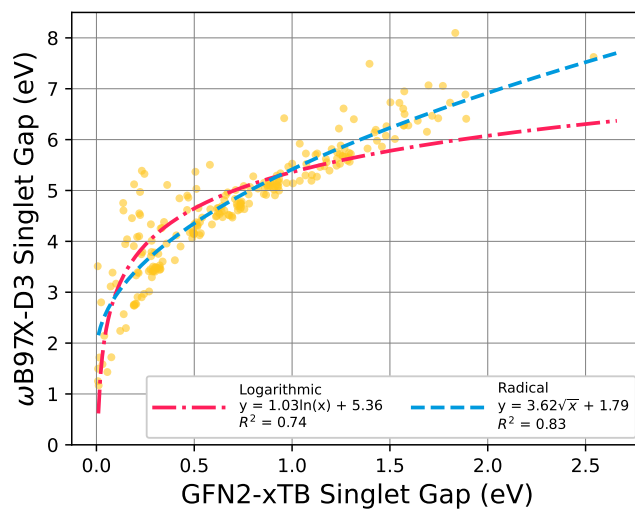


Figure S1: Correlation between HOMO-LUMO gaps calculated using GFN2-xTB versus ω B97X-D3. The logarithmic, in red dash-dotted line, and the radical, in blue dashed line, best-fit functions, with their respective equations and coefficient of determination (R^2), are shown.

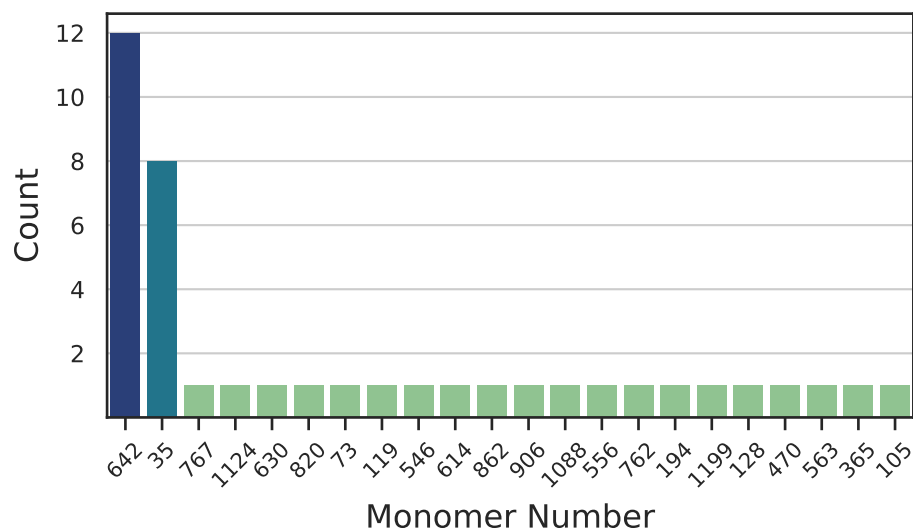


Figure S2: The number of times a monomer was part of the top 20 oligomers, i.e. with the lowest xTB-GNF2 HOMO-LUMO gap, found in all 10 GA runs. Each of the oligomers had either monomer 642 or monomer 35 as one of their monomers.

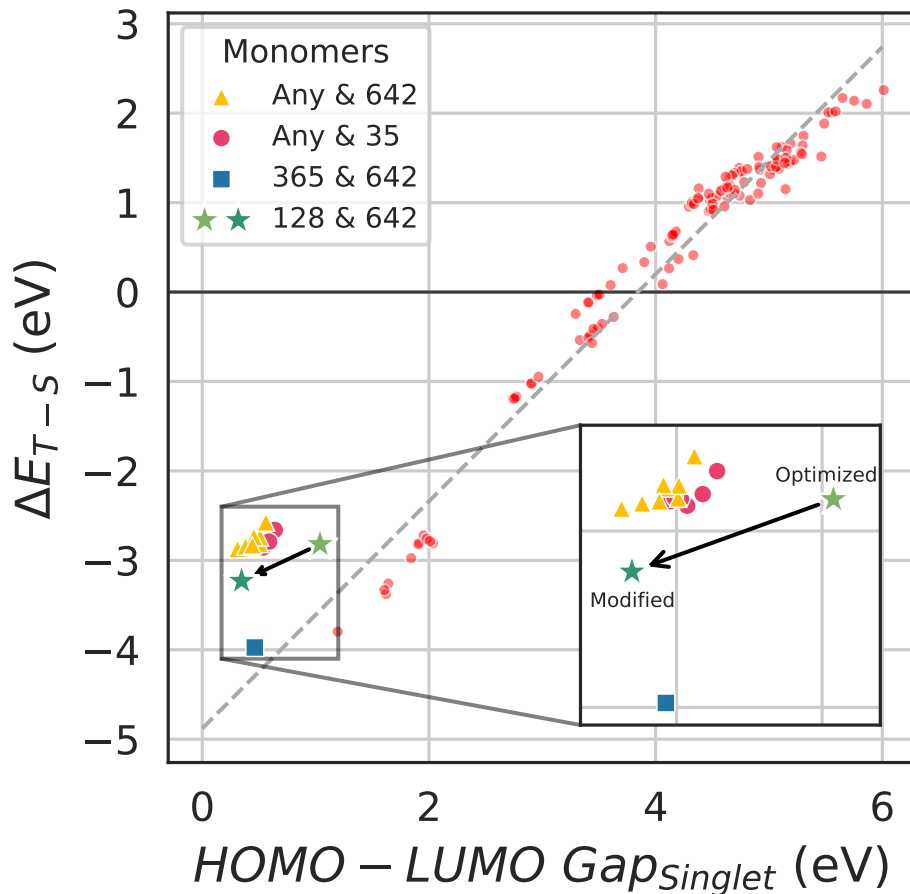


Figure S3: Correlation between the singlet HOMO-LUMO gap and ΔE_{T-S} of the 16 out of the top 20 oligomers. The oligomers are grouped by the common monomers—35 (in yellow triangles) and 624 (in pink circles). The outlier of monomer 128 and 642 is indicated with light green star with the values of its optimized geometry (at the arrow's tail) and with a dark green star at its values in the modified geometry (at the arrow's head). The outlier of monomers 365 and 642 is indicated in a blue square. A zoomed-in inset of the relevant part is shown. The red points are the data points from the previous study, with the best fit line for those points shown in dashed gray line.

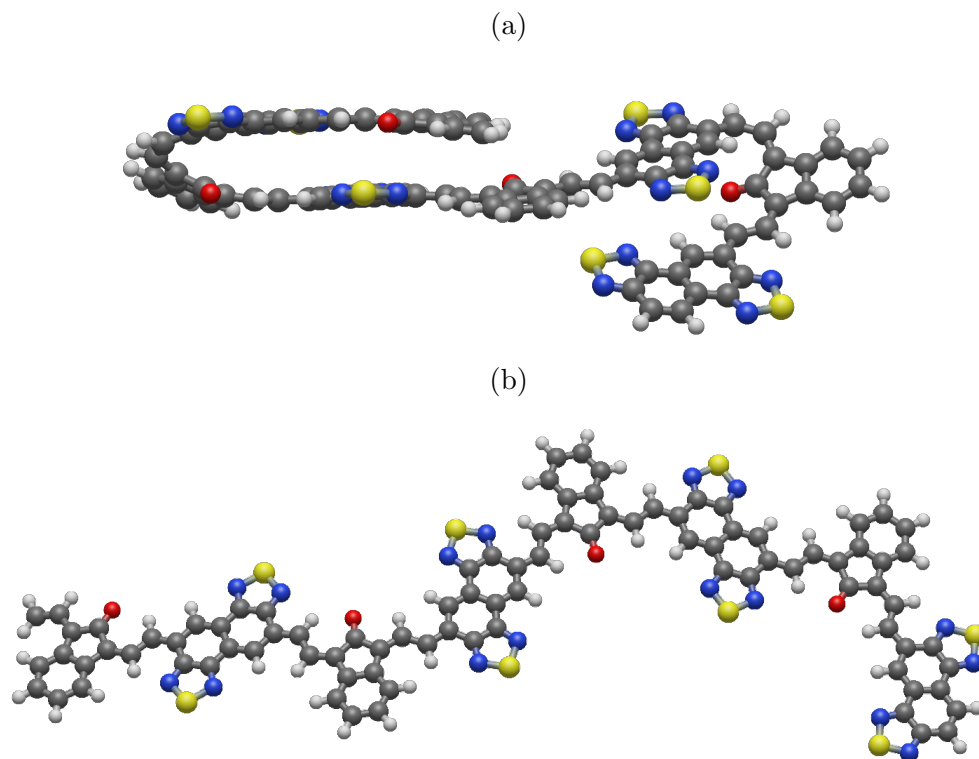


Figure S4: (a) A side view of the optimized, folded conformation of oligomer 128_642, (b) A top view of the modified, flat conformation of oligomer 128_642.

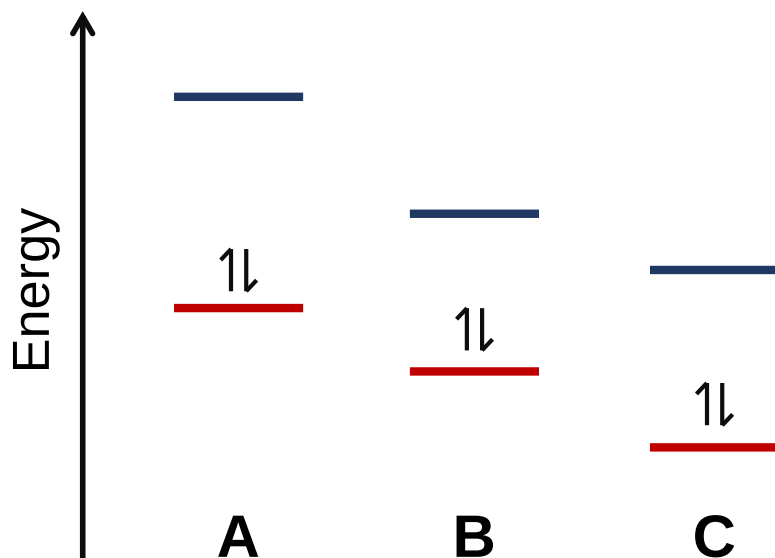
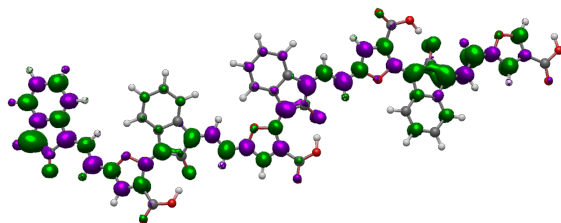
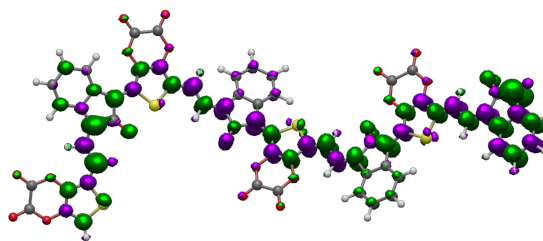


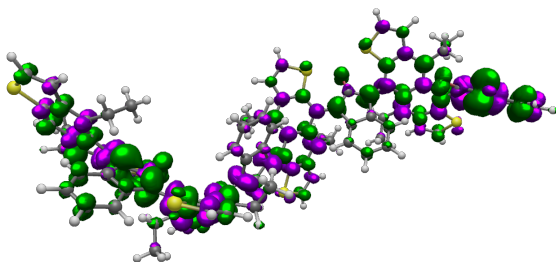
Figure S5: Relative HOMO (in red) and LUMO (in blue) levels of hypothetical monomers A, B, and C. If monomers A and B were to combine in a polymer monomer A will be the donor while monomer B will be the acceptor, as the HOMO level of monomer A is relatively higher in energy than monomer B. However, if monomers B and C were to combine to make a polymer then monomer B will be the donor while monomer C will be the acceptor. Monomer B can behave as either a donor or acceptor, depending on which monomer it is paired with.



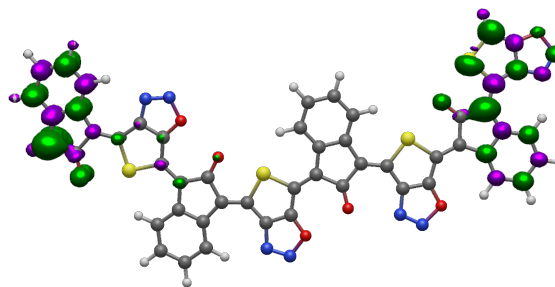
(a) 35-906



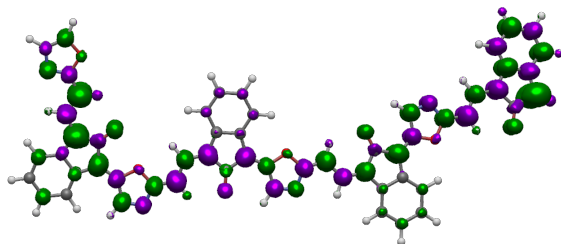
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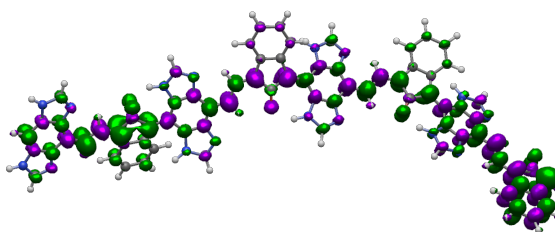
(c) 35-119



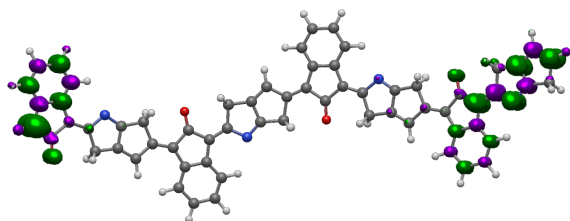
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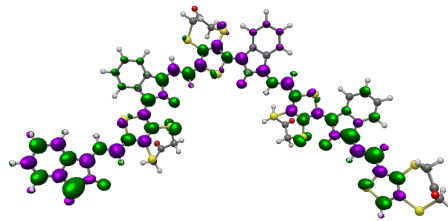
(e) 35-194



(f) 35-563

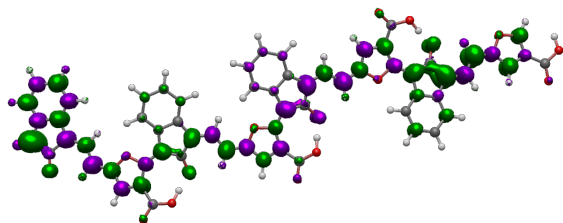


(g) 35-614

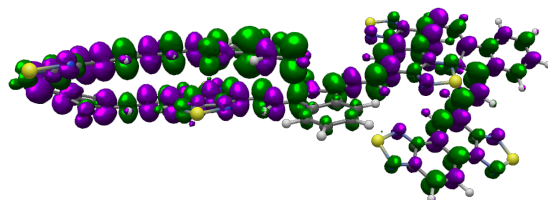


(h) 35-73

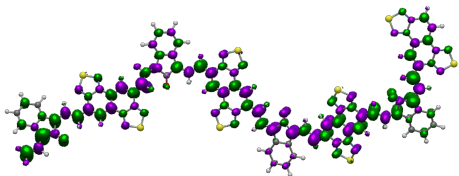
Figure S6: Spin density plots of the top 20 oligomers. Isosurface value is 0.002 a.u.



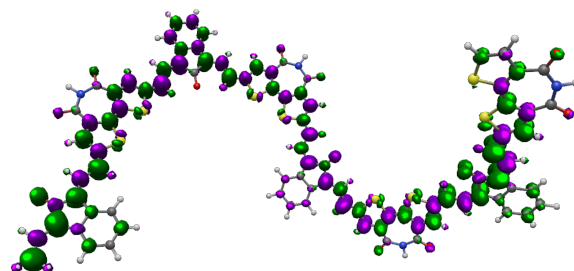
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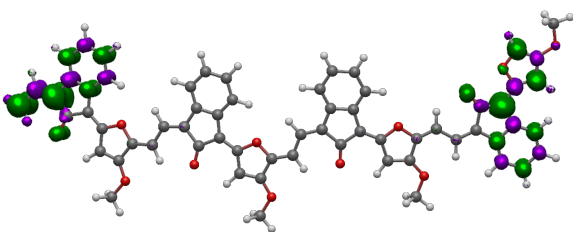
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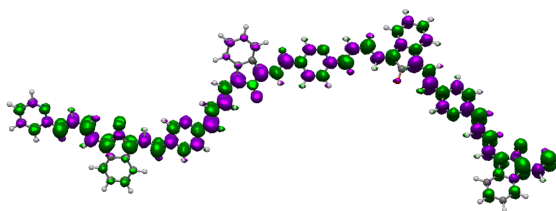
(k) 642-128 modified



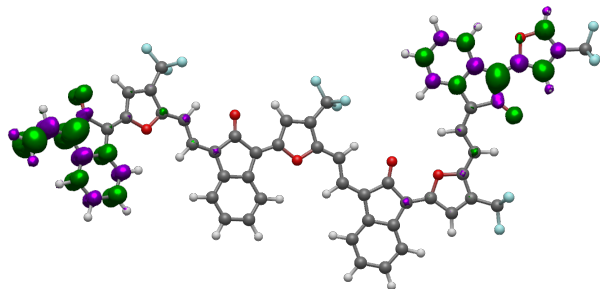
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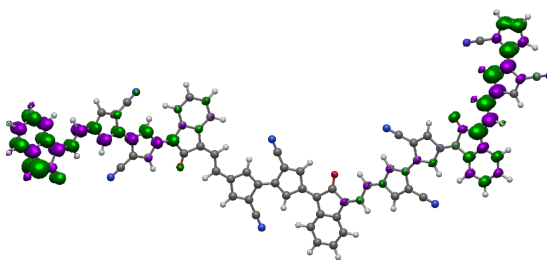
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(n) 642-546

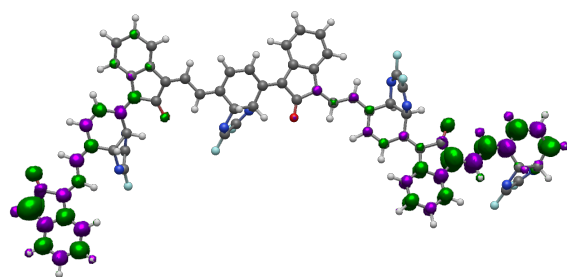


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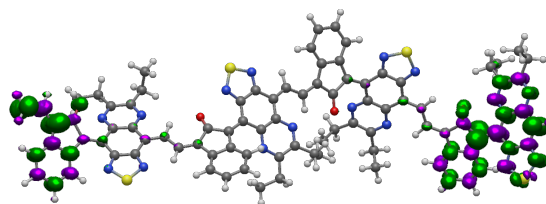


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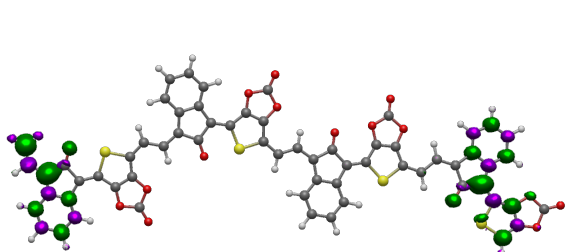
Figure S6: Cont. Spin density plots of the top 20 oligomers. Isosurface value is 0.002 a.u.



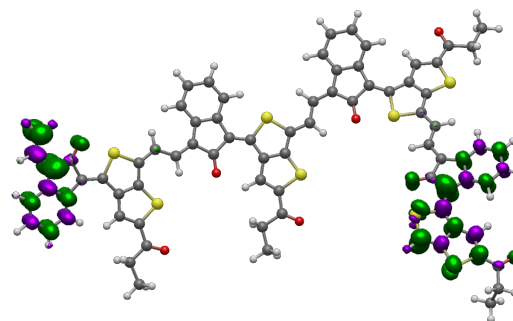
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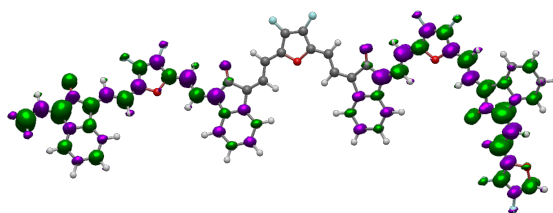
(r) 642-762



(s) 642-767



(t) 642-820



(u) 642-862

Figure S6: Cont. Spin density plots of the top 20 oligomers. Isosurface value is 0.002 a.u.

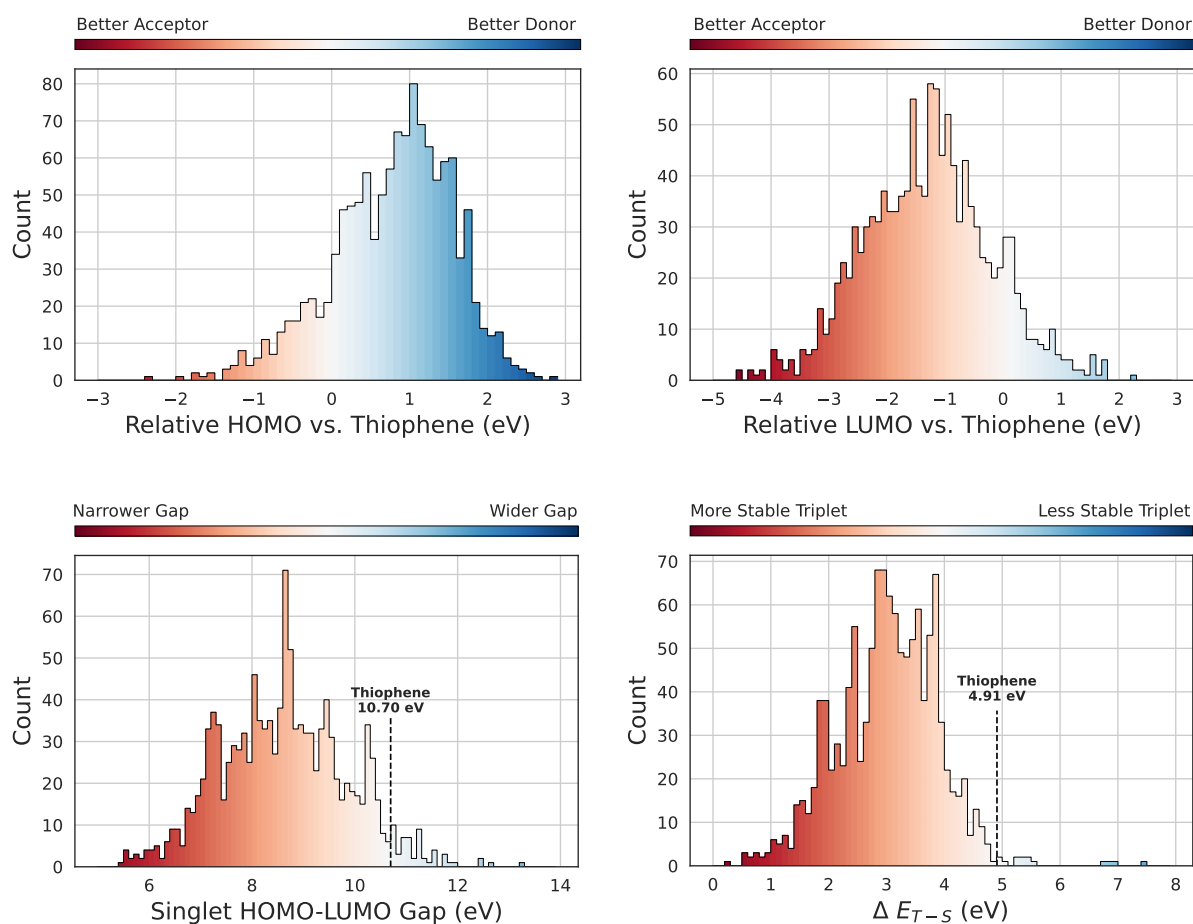


Figure S7: Top Left: a histogram of the monomers' HOMO eigenvalue relative to thiophene's HOMO eigenvalue. Top Right: a histogram of the monomers' LUMO eigenvalue relative to thiophene's LUMO eigenvalue. Bottom Left: A histogram of the monomers' HOMO-LUMO gap. Thiophene's HOMO-LUMO gap is marked for reference. Bottom Right: A histogram of the monomers' electronic energy difference between the triplet and singlet ground states. A Lower value correlates to a more stable triplet ground-state. Thiophene's ΔE_{T-S} is marked for reference.

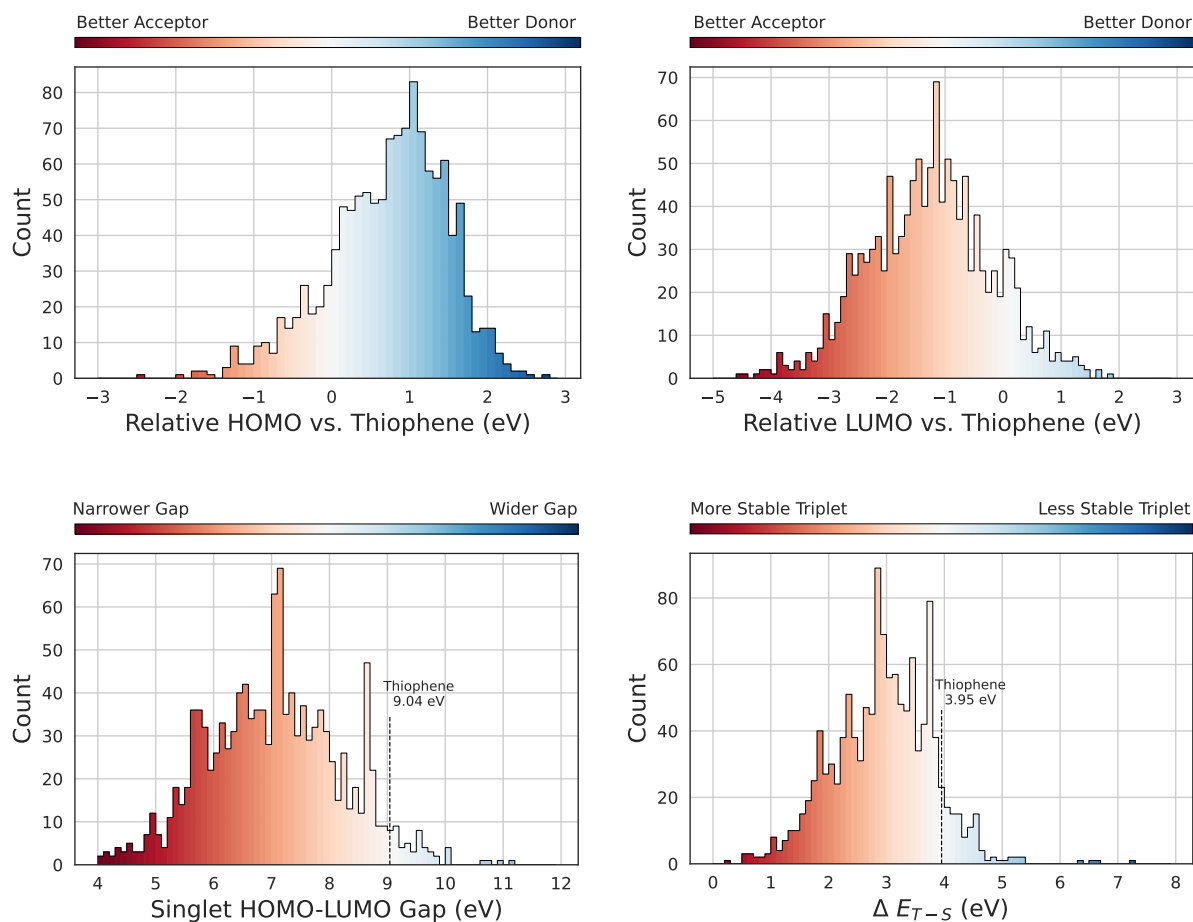


Figure S8: CAM-B3LYP single point calculations on the monomers that show similar distributions to the ω B97X-D3 single point calculations in Figure S7. Top Left: a histogram of the monomers' HOMO eigenvalue relative to thiophene's HOMO eigenvalue. Top Right: a histogram of the monomers' LUMO eigenvalue relative to thiophene's LUMO eigenvalue. Bottom Left: A histogram of the monomers' HOMO-LUMO gap. Thiophene's HOMO-LUMO gap is marked for reference. Bottom Right: A histogram of the monomers' electronic energy difference between the triplet and singlet ground states. A Lower value correlates to a more stable triplet ground-state. Thiophene's ΔE_{T-S} is marked for reference.

Table S1: The HOMO level (relative to thiophene's), LUMO level (relative to thiophene's), the HOMO-LUMO gap and the ΔE_{T-S} of the 10 most common monomers from all the GA runs (Figure 3).

Monomer	Relative HOMO	Relative LUMO	HOMO-LUMO Gap	ΔE_{T-S}
35	1.05	-3.35	6.31	0.71
77	1.71	-2.54	6.45	0.92
115	-0.87	-4.58	6.99	1.63
187	-0.19	-4.51	6.38	1.28
221	0.15	-3.35	7.20	1.13
642	1.56	-3.49	5.65	0.28
686	1.33	-2.51	6.86	1.60
778	2.65	-2.50	5.55	0.68
1029	-0.66	-3.62	7.74	3.41
1212	0.62	-3.69	6.38	1.17

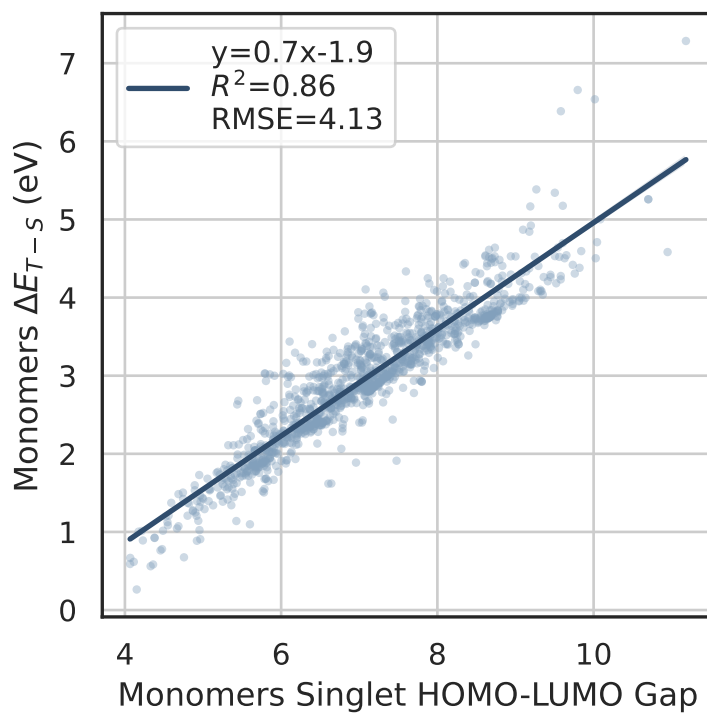


Figure S9: Correlation between the monomers' singlet HOMO-LUMO gap and the stability of their triplet ground state, ΔE_{T-S} .

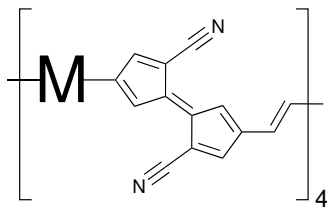


Figure S10: Visualization of the oligomers constructed by some monomer, **M**, and monomer number 630, for Figure 5.

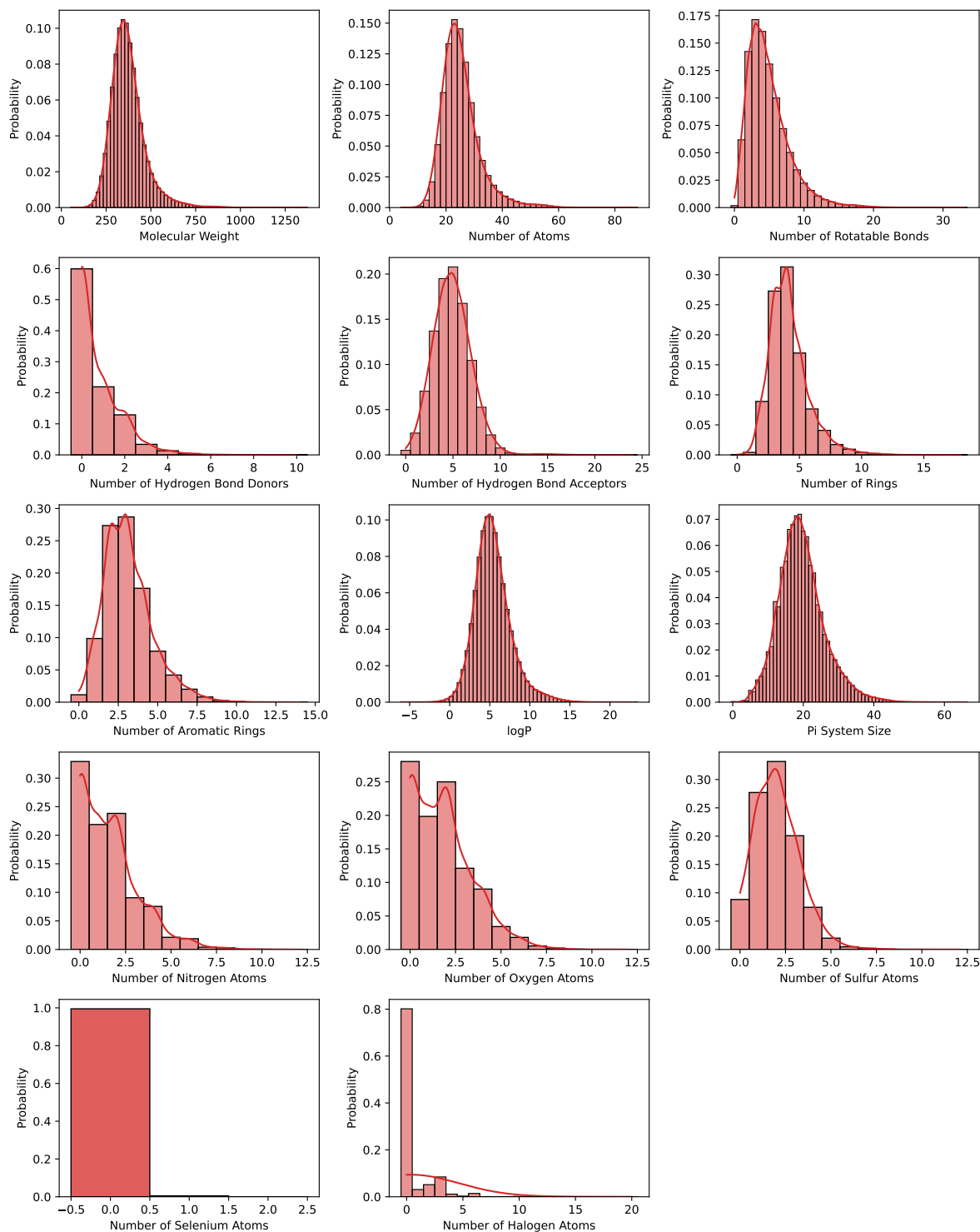


Figure S11: Various descriptors of all (~1.5 million) possible monomer pairs.

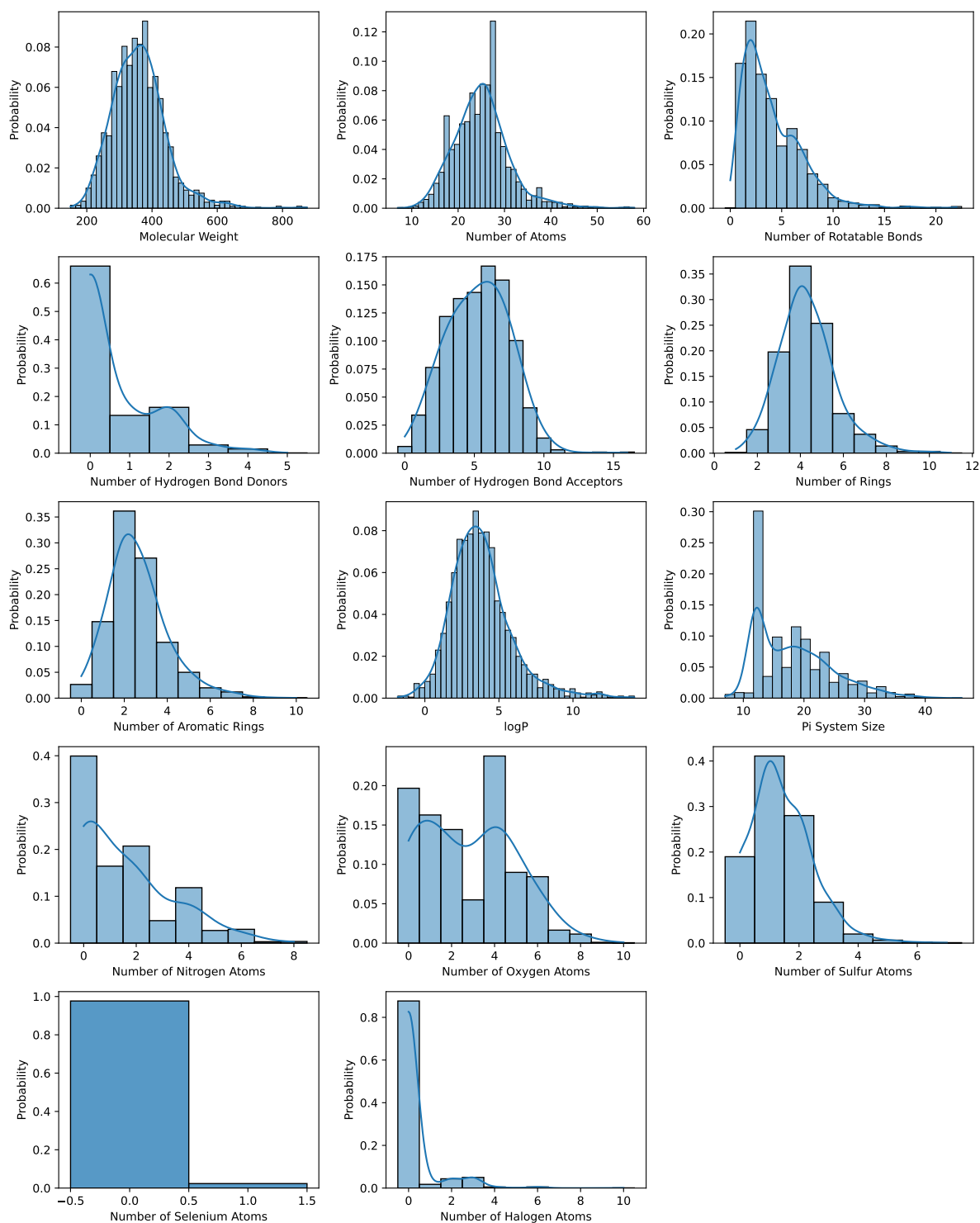


Figure S12: Various descriptors of the monomer pairs of the oligomers with GFN2-xTB-calculated HOMO-LUMO gap smaller than 0.2 eV that were generated in any of the GA runs.

Table S2: Full data for Figure 5. Monomers number that were combined with 630 to create an oligomer, each monomer's relative HOMO, relative LUMO, its singlet HOMO-LUMO gap and its ΔE_{T-S} , and the ΔE_{T-S} of the full oligomer. The table is sorted by the ascending oligomer's ΔE_{T-S} .

Monomer Number	Monomer Relative HOMO	Monomer Relative LUMO	Monomer Singlet Gap	Monomer ΔE_{T-S}	Oligomer ΔE_{T-S}
261	0.73	-3.46	6.51	1.05	-2.96
224	0.06	-4.26	6.37	1.29	-2.75
1172	1.66	-3.14	5.89	0.80	-2.72
768	1.77	-2.75	6.17	1.08	-2.70
141	1.92	1.19	9.97	3.98	-2.69
1064	2.29	-2.28	6.13	1.56	-2.42
1181	2.18	-2.33	6.18	1.21	-2.10
200	2.34	-2.29	6.06	1.54	-2.03
775	1.91	-3.20	5.59	0.64	-1.88
710	1.21	-2.24	7.24	1.92	-1.79
663	0.63	-2.04	8.04	2.48	-1.51
40	0.93	-1.98	7.78	2.38	-1.43
1027	1.16	-3.00	6.54	0.96	-1.06
630	0.14	-4.13	6.43	1.32	-1.00
1128	-0.41	-4.33	6.78	1.68	-1.00
337	0.76	-1.47	8.46	3.44	-0.99
913	2.48	-2.32	5.90	1.01	-0.93
1002	0.18	-0.40	10.12	3.46	-0.71
105	-0.33	-4.11	6.92	1.56	-0.70
639	0.58	-2.75	7.37	2.16	-0.46
804	1.06	-0.81	8.82	2.99	-0.33
75	2.59	-2.00	6.10	1.04	-0.30
730	1.46	-3.22	6.02	1.15	-0.15
728	1.74	-1.78	7.17	1.81	-0.14
1204	2.83	0.68	8.54	3.21	-0.08
1067	1.55	-3.49	5.66	0.91	-0.04
722	1.52	-3.13	6.04	1.11	-0.03
203	2.49	-2.43	5.78	0.56	0.01
569	1.09	-3.18	6.43	1.43	0.02
395	1.73	-3.48	5.50	0.55	0.04
697	1.31	-3.32	6.06	1.41	0.05
225	2.22	0.23	8.70	3.15	0.07
526	1.62	0.83	9.91	3.89	0.16
466	2.41	-2.76	5.53	1.06	0.19
1054	0.26	-1.05	9.39	3.57	0.20
332	-0.52	-4.30	6.92	1.62	0.21
305	2.55	-2.35	5.81	0.58	0.23

Table S2, cont'd

Monomer Number	Monomer Relative HOMO	Monomer Relative LUMO	Monomer Singlet Gap	Monomer ΔE_{T-S}	Oligomer ΔE_{T-S}
210	2.37	-0.28	8.04	3.06	0.23
137	-0.08	-3.91	6.87	1.67	0.32
176	2.36	-2.76	5.58	1.07	0.35
588	1.29	-1.90	7.50	2.76	0.35
670	2.23	-1.06	7.41	2.36	0.39
418	2.24	-0.72	7.74	2.48	0.40
503	0.20	-3.99	6.51	1.67	0.41
34	1.93	-0.22	8.55	3.26	0.46
349	0.24	-3.97	6.49	1.57	0.47
954	2.25	1.01	9.45	3.85	0.50
343	2.18	-2.81	5.71	0.89	0.51
534	-0.22	-1.91	9.01	3.13	0.53
100	0.48	-0.78	9.44	3.57	0.56
104	2.22	-2.77	5.71	0.88	0.58
618	0.04	-2.01	8.65	2.95	0.62
389	-0.97	-2.11	9.56	3.65	0.63
457	-1.14	-1.62	10.22	3.85	0.63
869	-1.34	-1.93	10.11	3.80	0.65
1	1.45	0.65	9.90	3.90	0.65
723	-1.28	-1.88	10.10	5.27	0.67
591	-1.19	-1.26	10.63	4.07	0.69
1203	-1.35	-2.08	9.96	3.82	0.71
764	0.72	-2.57	7.40	2.34	0.71
472	-1.59	-2.57	9.72	3.82	0.72
0	-1.23	-1.18	10.74	4.13	0.76
160	0.14	-3.80	6.76	1.50	0.76
976	-1.64	-2.61	9.72	4.24	0.79
5	0.04	-3.76	6.89	1.88	0.80
41	0.05	-1.51	9.14	1.95	0.82
1071	1.40	-1.29	8.00	3.28	0.87
242	0.85	-1.01	8.84	4.20	0.88
515	-1.37	-2.58	9.48	3.75	0.89
1030	-1.20	-2.47	9.42	3.58	0.90
826	1.34	-1.29	8.06	2.46	0.90
519	-1.27	-0.13	11.84	5.09	0.91
413	0.96	1.52	11.25	4.62	0.93
966	-1.10	-3.79	8.00	3.25	0.95
471	1.74	-1.79	7.16	1.82	0.96
1136	-1.71	-1.27	11.13	4.36	0.97
893	-0.99	-3.82	7.86	3.27	0.98
746	0.72	1.14	11.12	4.37	0.99
346	-0.77	-3.85	7.62	3.00	0.99
783	0.36	-0.51	9.83	3.59	1.03
1135	-1.21	-1.17	10.74	4.39	1.04

Table S2, cont'd

Monomer Number	Monomer Relative HOMO	Monomer Relative LUMO	Monomer Singlet Gap	Monomer ΔE_{T-S}	Oligomer ΔE_{T-S}
996	1.48	-2.22	6.99	1.81	1.06
1095	0.47	-2.04	8.18	2.80	1.06
943	0.64	-2.74	7.32	2.10	1.07
67	1.65	0.58	9.64	3.85	1.08
725	-2.39	-3.87	9.22	3.61	1.08
533	0.27	0.84	11.27	4.31	1.08
581	-1.55	-3.94	8.30	3.32	1.09
504	1.00	1.38	11.07	4.11	1.10
190	-1.75	-3.91	8.54	3.46	1.10
809	1.08	-2.09	7.52	2.06	1.10
673	-1.11	0.89	12.70	4.66	1.10
1000	-1.16	0.57	12.43	5.36	1.10
20	-1.19	-2.19	9.70	4.02	1.11
450	1.65	-1.05	8.00	2.51	1.11
156	0.60	0.07	10.17	4.40	1.13
1063	1.32	-1.43	7.95	2.89	1.13
672	0.87	1.70	11.53	4.68	1.14
345	1.10	-2.39	7.21	1.87	1.14
665	0.88	-1.14	8.68	2.70	1.16
435	0.49	-2.14	8.07	2.42	1.17
257	1.54	1.79	10.95	4.46	1.18
1131	-1.95	-2.64	10.00	4.11	1.18
1216	1.50	-2.02	7.18	2.11	1.18
538	1.26	1.00	10.43	4.60	1.18
440	0.18	-2.36	8.15	3.53	1.19
805	0.93	-1.13	8.64	3.10	1.19
1072	0.66	1.75	11.79	6.98	1.19
694	-0.47	-1.15	10.01	3.69	1.19
3	1.79	-1.95	6.95	1.76	1.19
117	0.49	-1.09	9.12	3.28	1.20
1035	-1.16	0.57	12.43	5.36	1.21
1142	-0.02	-0.66	10.06	4.10	1.21
521	0.43	1.72	11.98	6.85	1.23
1126	-0.57	-2.07	9.19	3.50	1.26
416	1.29	1.61	11.02	5.50	1.28
206	0.59	-0.91	9.19	3.50	1.28
51	0.28	-0.16	10.26	3.79	1.29
360	1.07	-0.91	8.72	2.89	1.29
151	0.91	-0.41	9.37	3.36	1.29
507	0.00	0.00	10.70	4.91	1.29
322	-0.25	2.29	13.23	7.44	1.30
182	-0.35	0.23	11.27	4.57	1.30
1116	0.93	-0.14	9.63	3.69	1.31
819	-0.10	-0.49	10.31	4.72	1.31

Table S2, cont'd

Monomer Number	Monomer Relative HOMO	Monomer Relative LUMO	Monomer Singlet Gap	Monomer ΔE_{T-S}	Oligomer ΔE_{T-S}
947	1.59	-1.23	7.87	2.65	1.31
499	-0.50	-0.36	10.84	4.97	1.31
559	0.66	-1.16	8.88	3.03	1.32
288	0.97	-0.67	9.06	3.39	1.32
932	2.03	-1.35	7.32	2.67	1.32
78	0.47	1.11	11.33	4.61	1.32
587	1.51	-2.67	6.52	1.31	1.33
1094	2.12	1.14	9.72	3.59	1.33
766	-0.77	-0.95	10.52	5.43	1.34
874	0.97	-1.42	8.30	2.94	1.34
698	0.07	-1.53	9.10	3.23	1.35
900	-0.45	0.38	11.53	4.46	1.35
425	0.65	0.24	10.29	4.24	1.38
393	0.97	-1.12	8.61	3.00	1.38
542	-0.21	-0.53	10.38	4.74	1.40
28	1.07	-2.80	6.83	1.85	1.41
467	-0.34	0.44	11.48	4.39	1.41
981	1.27	1.53	10.95	4.29	1.42
987	0.09	-1.55	9.06	3.48	1.43
784	1.52	-1.06	8.11	3.02	1.43
555	1.12	1.38	10.95	4.22	1.43
1090	-0.86	-3.15	8.41	3.46	1.44
444	0.74	-1.78	8.17	2.89	1.46
79	0.96	-1.01	8.73	2.89	1.46
310	0.15	-1.04	9.51	3.57	1.47
350	0.90	-1.06	8.74	3.46	1.47
412	0.43	0.15	10.41	3.87	1.47
468	-0.35	-2.45	8.60	2.98	1.48
1118	1.67	0.01	9.04	3.44	1.48
249	0.74	1.55	11.51	5.29	1.48
292	0.17	-0.51	10.02	3.90	1.49
979	0.50	1.02	11.22	5.43	1.51
552	1.67	0.44	9.46	3.58	1.53
439	-0.87	0.13	11.70	4.58	1.55
724	0.46	1.01	11.25	4.74	1.59
473	1.24	-0.34	9.11	3.70	1.61
898	-0.34	-2.37	8.67	2.92	1.62
687	1.56	-0.69	8.45	2.94	1.67
983	1.59	-1.99	7.12	1.93	1.94
226	1.51	-0.12	9.06	3.18	2.02
659	1.08	-1.59	8.03	2.43	2.03

Table S3: Monomers number and structure.

Number	Structure
0	
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Table S3, cont'd

Number	Structure
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Table S3, cont'd

Number	Structure
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Table S3, cont'd

Number	Structure
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Table S3, cont'd

Number	Structure
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Table S3, cont'd

Number	Structure
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Table S3, cont'd

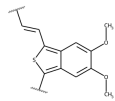
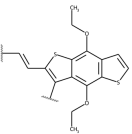
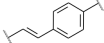
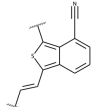
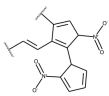
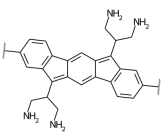
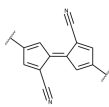
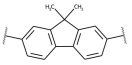
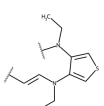
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Table S3, cont'd

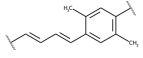
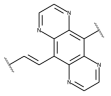
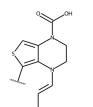
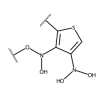
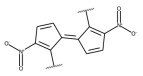
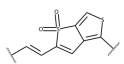
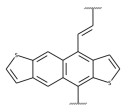
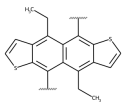
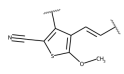
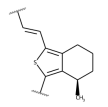
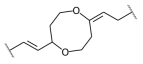
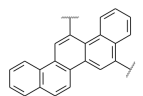
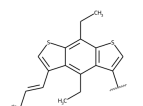
Number	Structure
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Table S3, cont'd

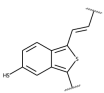
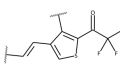
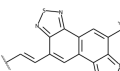
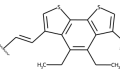
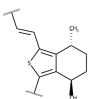
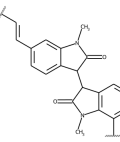
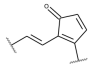
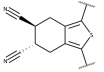
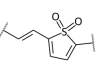
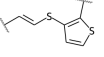
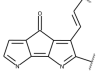
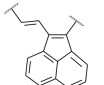
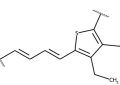
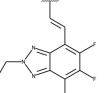
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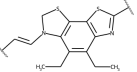
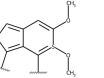
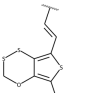
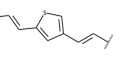
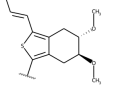
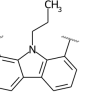
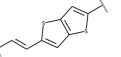
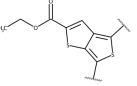
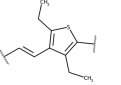
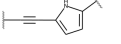
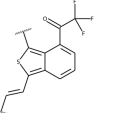
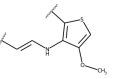
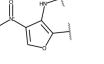
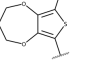
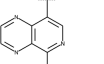
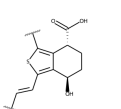
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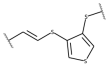
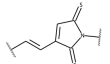
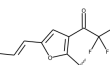
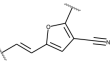
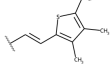
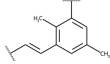
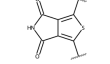
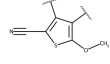
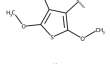
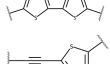
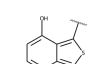
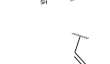
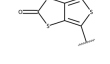
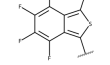
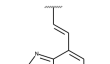
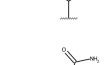
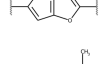
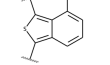
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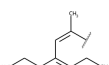
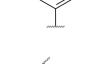
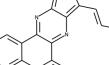
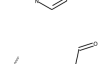
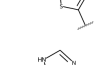
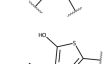
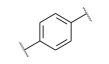
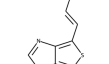
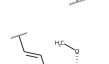
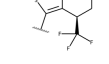
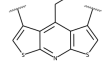
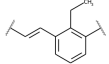
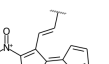
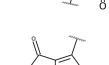
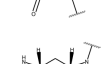
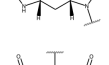
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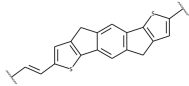
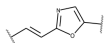
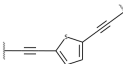
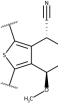
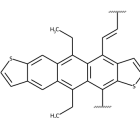
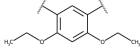
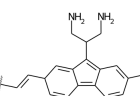
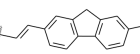
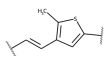
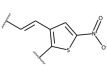
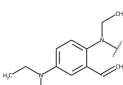
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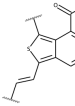
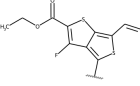
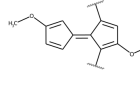
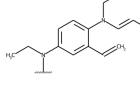
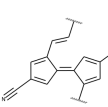
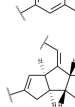
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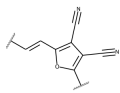
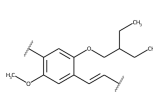
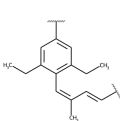
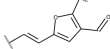
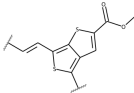
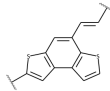
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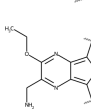
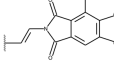
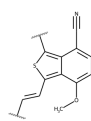
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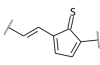
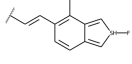
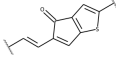
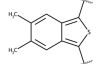
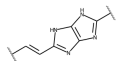
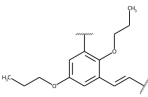
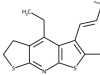
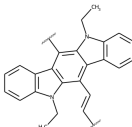
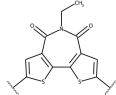
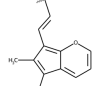
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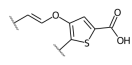
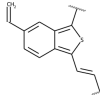
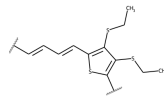
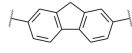
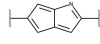
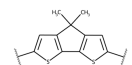
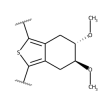
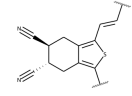
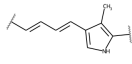
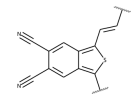
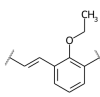
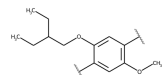
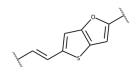
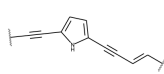
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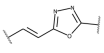
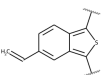
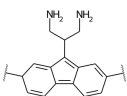
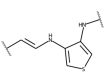
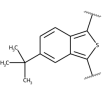
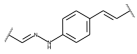
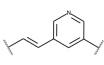
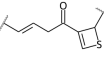
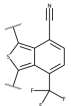
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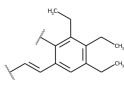
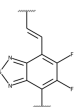
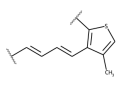
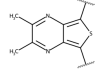
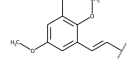
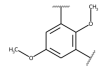
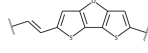
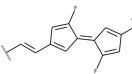
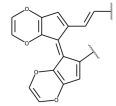
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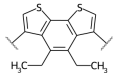
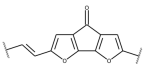
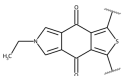
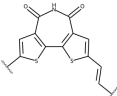
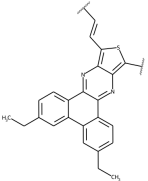
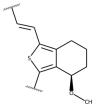
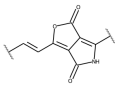
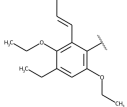
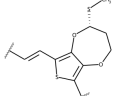
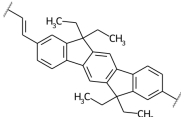
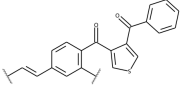
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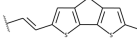
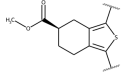
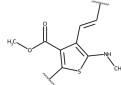
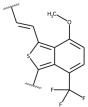
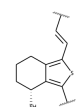
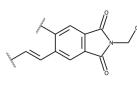
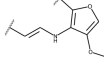
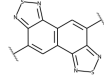
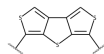
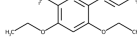
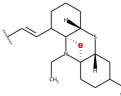
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Table S3, cont'd

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Table S3, cont'd

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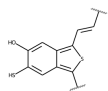
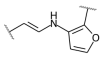
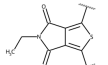
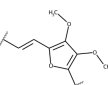
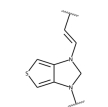
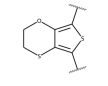
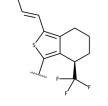
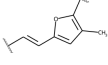
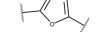
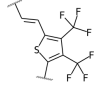
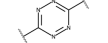
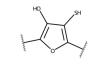
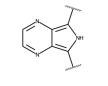
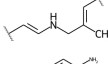
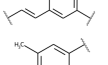
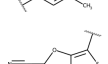
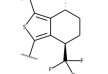
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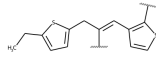
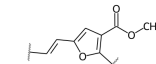
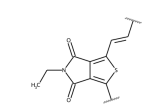
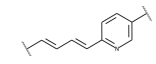
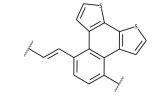
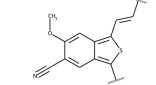
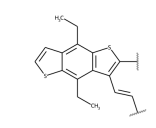
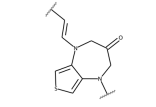
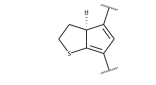
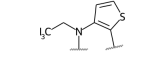
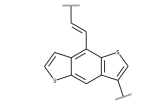
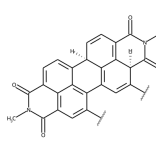
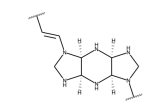
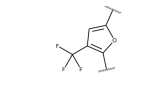
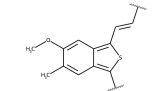
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Table S3, cont'd

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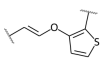
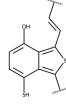
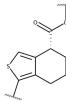
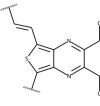
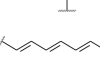
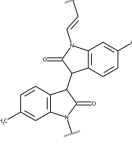
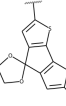
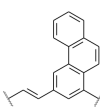
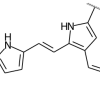
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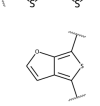
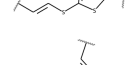
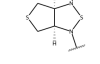
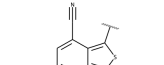
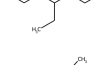
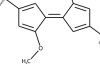
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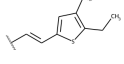
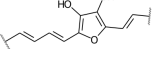
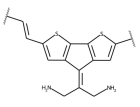
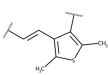
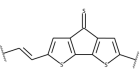
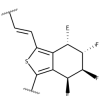
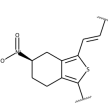
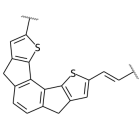
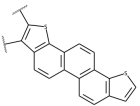
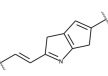
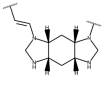
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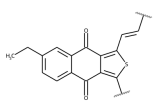
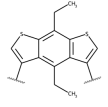
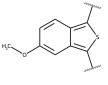
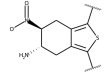
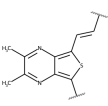
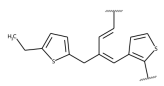
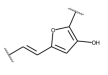
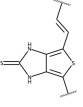
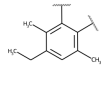
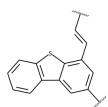
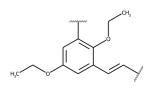
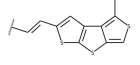
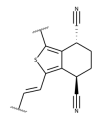
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Table S3, cont'd

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Table S3, cont'd

Number	Structure
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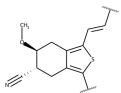
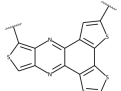
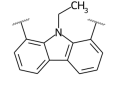
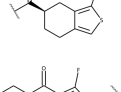
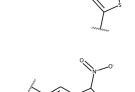
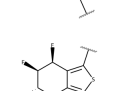
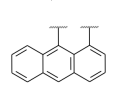
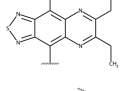
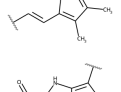
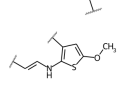
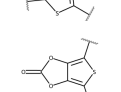
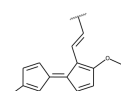
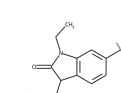
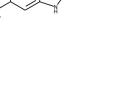
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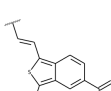
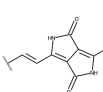
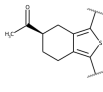
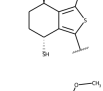
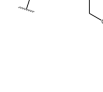
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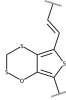
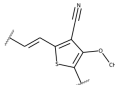
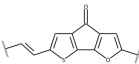
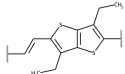
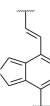
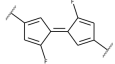
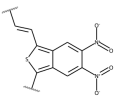
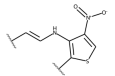
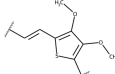
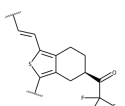
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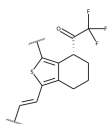
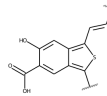
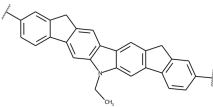
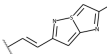
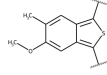
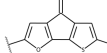
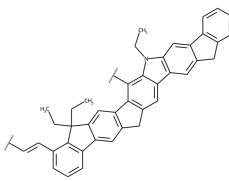
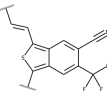
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Table S3, cont'd

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Table S3, cont'd

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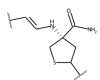
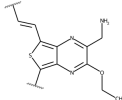
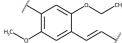
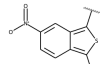
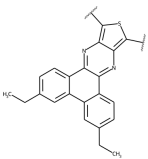
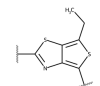
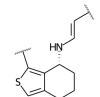
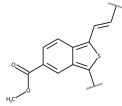
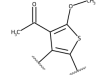
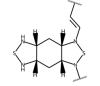
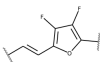
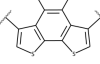
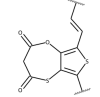
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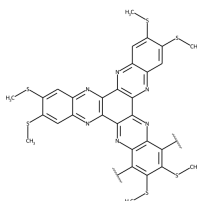
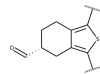
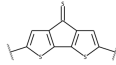
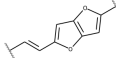
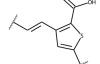
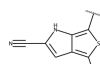
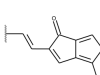
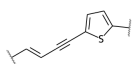
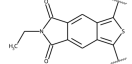
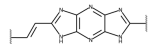
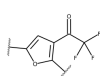
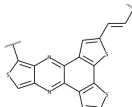
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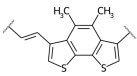
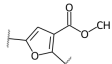
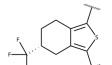
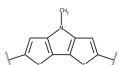
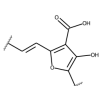
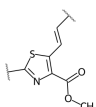
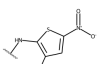
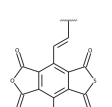
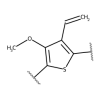
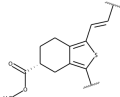
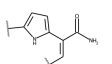
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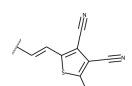
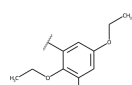
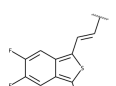
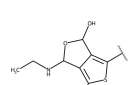
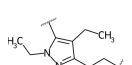
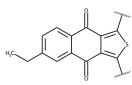
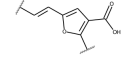
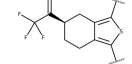
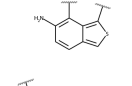
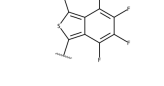
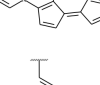
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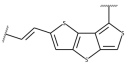
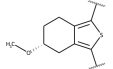
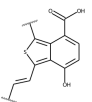
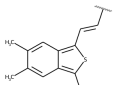
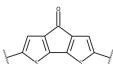
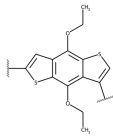
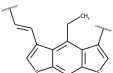
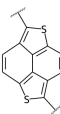
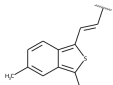
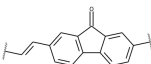
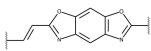
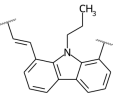
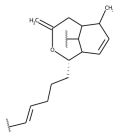
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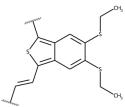
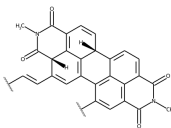
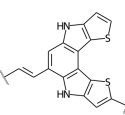
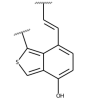
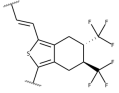
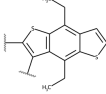
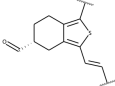
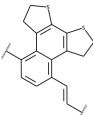
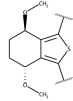
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Table S3, cont'd

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Table S3, cont'd

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Table S3, cont'd

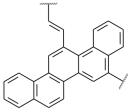
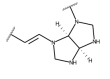
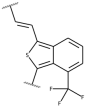
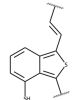
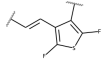
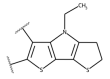
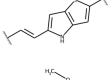
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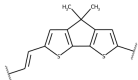
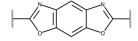
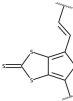
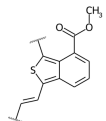
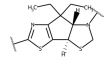
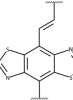
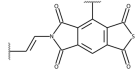
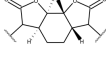
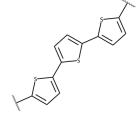
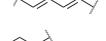
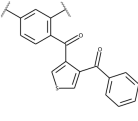
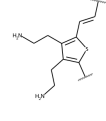
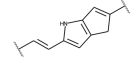
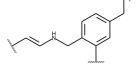
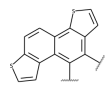
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Table S3, cont'd

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Table S3, cont'd

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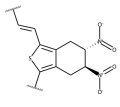
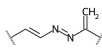
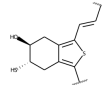
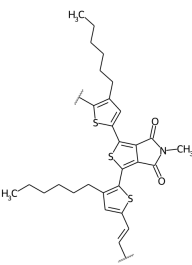
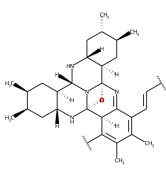
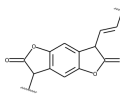
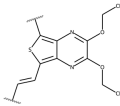
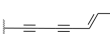
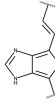
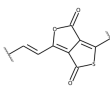
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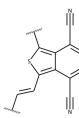
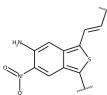
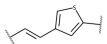
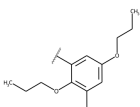
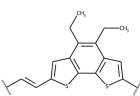
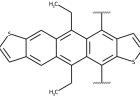
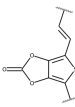
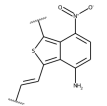
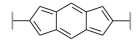
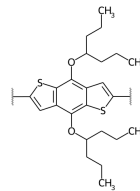
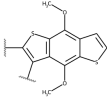
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Table S3, cont'd

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Table S3, cont'd

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