Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

A time and resource efficient machine learning assisted design of non-fullerene small molecule acceptors for P3HT-based organic solar cells and green solvent selection

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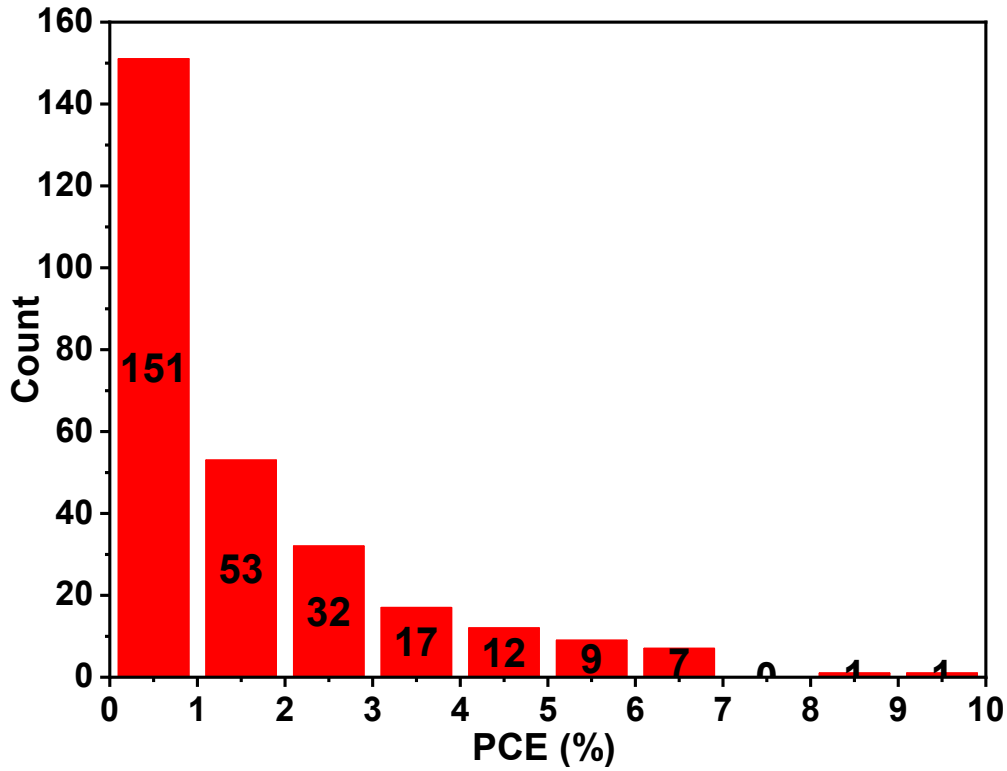


Fig. S1. Distribution of experimental efficiencies of P3HT-based OSC in the data set.

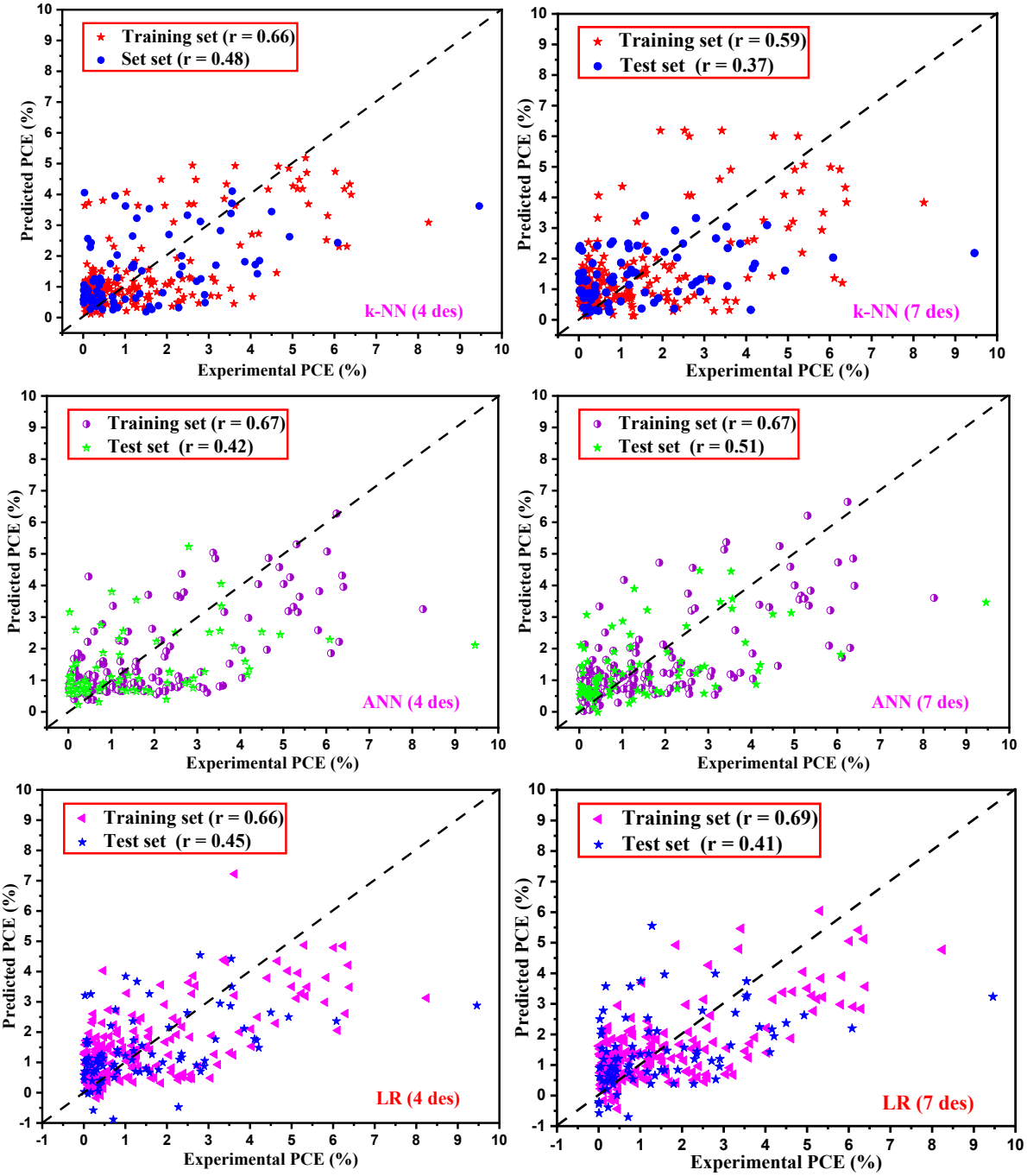


Fig. S2. Pearson correlation between experimental PCE and predicted PCE calculated through k-nearest neighbor (k-NN), artificial neural network (ANN) and linear regression (LR) using 4 and 7 descriptors.

Table S1. Difference between experimental and predicted HOMO and LUMO values for NFAs not included in training and test sets.

No	Acceptor	Exp. HOMO	Pred. HOMO	Diff	Exp. LUMO	Pred. LUMO	Diff.	Ref.

		(eV)	(eV)		(eV)	(eV)		
1	CDTCN	-5.39	-5.41	0.02	-3.80	-3.73	0.07	[1]
2	FOC6-IC	-5.42	-5.42	0.00	-3.77	-3.79	0.02	[2]
3	FOC6-FIC	-5.47	-5.46	0.01	-3.81	-3.89	0.08	[2]
4	cis-PolyPBI	-5.82	-5.78	0.04	-3.79	-3.82	0.03	[3]
5	NTIC-OMe	-5.53	-5.47	0.06	-3.70	-3.72	0.02	[4]
6	NTIC-F	-5.52	-5.49	0.03	-3.77	-3.77	0.00	[4]
7	DTFT5-FIC	-5.52	-5.47	0.05	-3.87	-3.88	0.01	[5]
8	BTTPC	-5.47	-5.51	0.04	-3.78	-3.81	0.03	[6]
9	IDTV-ThIC	-5.43	-5.38	0.05	-3.72	-3.71	0.01	[7]
10	BCDT-4F	-5.46	-5.50	0.04	-3.86	-3.79	0.07	[8]
11	NFTI	-5.46	-5.41	0.05	-3.77	-3.78	0.01	[9]
12	ITOM1	-5.5	-5.43	0.07	-3.76	-3.73	0.03	[10]
13	ITOM4	-5.49	-5.44	0.05	-3.81	-3.75	0.06	[10]
14	ITThC	-5.47	-5.43	0.04	-3.76	-3.76	0.00	[11]
15	FDICTF	-5.43	-5.50	0.07	-3.71	-3.76	0.05	[12]
16	FDNCTF	-5.42	-5.49	0.07	-3.73	-3.73	0.00	[13]
17	O-NTIC	-5.51	-5.51	0.00	-3.67	-3.75	0.08	[14]
18	O-NTNC	-5.54	-5.51	0.01	-3.78	-3.74	0.04	[14]
19	Y9	-5.59	-5.50	0.04	-3.78	-3.75	0.03	[15]
20	IDTT-T	-5.52	-5.44	0.06	-3.54	-3.56	0.02	[16]

Table S2. Experimental and DFT calculated HOMO and LUMO values of NFAs

No.	Exp. HOMO (eV)	Calc. HOMO (eV)	Diff.	Exp. LUMO (eV)	Calc. LUMO (eV)	Diff.	Method	Ref.
1	-5.56	-4.98	0.58	-3.81	-2.91	0.9	B3LYP/6-31G(d)	[17]
2	-5.7	-6.83	1.13	-3.99	-1.34	2.65	B3LYP/6-31G(d)	[17]
3	-5.5	-5.56	0.06	-3.25	-2.94	0.31	B3LYP/6-31G*	[18]
4	-5.55	-5.86	0.31	-3.29	-3.26	0.03	B3LYP/6-31G*	[18]
5	-6.07	-5.82	0.25	-3.96	-3.05	0.91	B3LYP/6-31g+(d,p)	[19]
6	-6.14	-5.87	0.27	-4.21	-3.65	0.56	B3LYP/6-31g+(d,p)	[19]
7	-5.52	-4.55	0.97	-3.86	-2.7	1.16	B3LYP/6-	[20]

							31G(d,p)	
8	-5.46	-4.56	0.9	-3.81	-2.72	1.09	B3LYP/6-31G(d,p)	[20]
9	-5.64	-5.08	0.56	-3.99	-3.3	0.69	B3LYP/6-31G(d,p)	[20]
10	-5.51	-5.2	0.31	-3.55	-3.13	0.42	B3LYP/6-31G	[21]
11	-5.43	-5.12	0.31	-3.38	-2.95	0.43	B3LYP/6-31G	[22]
12	-5.6	-6.03	0.429	-3.03	-2.98	0.05	B3LPY/6-311+G(d)	[23]
13	-5.92	-6.18	0.258	-2.98	-2.97	0.01	B3LPY/6-311+G(d)	[23]
14	-5.23	-5.53	0.299	-3.44	-3.42	0.02	B3LPY/6-311+G(d)	[23]
15	-5.47	-5.77	0.299	-3.64	-3.42	0.22	B3LPY/6-311+G(d)	[23]
16	-5.92	-6.45	0.533	-3.82	-3.94	0.119	B3LPY/6-311+G(d)	[23]
17	-5.69	-6.18	0.494	-3.9	-3.94	0.039	B3LPY/6-311+G(d)	[23]
18	-5.66	-6.02	0.356	-3.29	-3.47	0.178	B3LPY/6-311+G(d)	[23]
19	-6	-6.29	0.29	-3.4	-3.65	0.25	B3LYP/6-31G(d,p)	[24]
20	-5.8	-5.76	0.04	-3.3	-3.15	0.15	B3LYP/6-31G(d,p)	[24]
21	-5.7	-5.77	0.07	-3.4	-3.27	0.13	B3LYP/6-31G(d,p)	[24]
22	-6.09	-5.87	0.22	-4.09	-3.48	0.61	B3LYP/6-31G**	[25]
23	-6.14	-5.88	0.26	-4.08	-3.48	0.6	B3LYP/6-31G**	[25]
24	-6.19	-5.94	0.25	-4.08	-3.49	0.59	B3LYP/6-31G**	[25]
25	-5.93	-5.24	0.69	-3.78	-3.35	0.43	B3LYP/6-31G	[26]
26	-5.68	-5.23	0.45	-3.81	-3.26	0.55	B3LYP/6-31G	[26]
27	-5.57	-5.49	0.08	-3.95	-3.14	0.81	B3LYP/6-31G	[26]
28	-5.81	-5.46	0.35	-3.99	-3.46	0.53	B3LYP/6-31G*	[27]
29	-5.4	-5.04	0.36	-3.65	-3.07	0.58	B3LYP/6-31G(d,p)	[28]
30	-5.4	-5	0.4	-3.61	-3.05	0.56	B3LYP/6-	[28]

							31G(d,p)	
31	-6.1	-6	0.1	-4.3	-3.5	0.8	B3LYP/6-31G(d,p)	[28]
32	-5.42	-5.18	0.24	-3.68	-3.25	0.43	B3LYP/6-31G	[29]
33	-5.63	-5.27	0.36	-3.59	-3.15	0.44	B3LYP/6-31G(d,p)	[29]
34	-5.32	-4.98	0.34	-3.23	-2.81	0.42	B3LYP/6-31G	[30]
35	-5.41	-5.05	0.36	-3.55	-2.99	0.56	B3LYP/6-31G	[30]
36	-5.37	-5.21	0.16	-3.64	-3.18	0.46	B3LYP/6-31G	[30]
37	-5.31	-5.34	0.03	-3.44	-3.17	0.27	B3LYP/6-31G (d, p)	[31]
38	-5.31	-5.41	0.1	-3.42	-3.28	0.14	B3LYP/6-31G	[31]
39	-5.62	-6.06	0.44	-3.65	-3.78	0.13	B3LYP/6-31G(d)	[32]
40	-5.46	-5.36	0.1	-3.61	-3.41	0.2	B3LYP/ 6-31G	[33]
41	-5.48	-5.56	0.08	-3.44	-2.97	0.47	B3LYP/6-31G(d)	[34]
42	-5.62	-5.76	0.14	-3.42	-2.96	0.46	B3LYP/6-31G(d)	[34]
43	-5.54	-5.67	0.13	-3.46	-2.83	0.63	B3LYP/6-31G(d)	[34]
44	-6.25	-6.18	0.07	-4.14	-3.67	0.47	B3LYP/6-31G(d,p)	[35]
45	-6.05	-6.1	0.05	-4.13	-3.64	0.49	B3LYP/6-31G(d,p)	[35]
46	-5.69	-5.79	0.1	-4.28	-3.9	0.38	B3LYP/6-31G(d,p)	[35]
47	-5.15	-4.69	0.46	-3.65	-2.8	0.85	B3LYP/6–31G	[36]
48	-5.2	-4.7	0.5	-3.74	-2.81	0.93	B3LYP/6–31G	[36]
49	-5.25	-4.88	0.37	-3.68	-2.88	0.8	B3LYP/6–31G	[36]
50	-5.33	-4.89	0.44	-3.61	-2.89	0.72	B3LYP/6–31G	[36]
51	-5.01	-5.15	0.14	-3.4	-2.91	0.49	B3LYP/6-31G(d)	[37]
52	-5.08	-5.38	0.3	-3.62	-3.4	0.22	B3LYP/6-31G(d)	[37]
53	-5.44	-4.71	0.73	-3.44	-2.81	0.63	B3LYP/6-	[38]

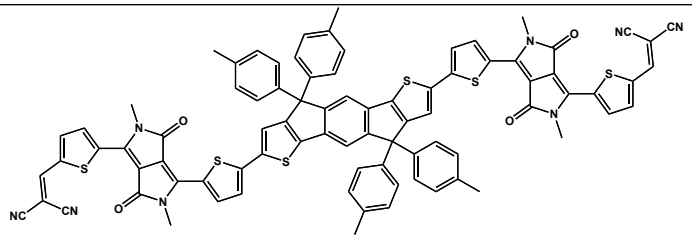
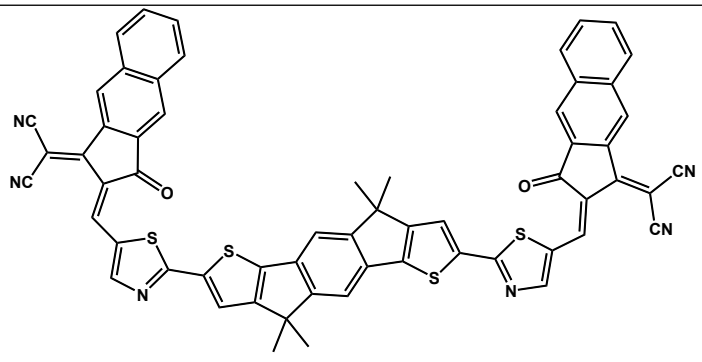
							31G(d,p)	
54	-5.3	-4.54	0.76	-3.41	-2.76	0.65	B3LYP/6-31G(d,p)	[38]
55	-5.42	-4.81	0.61	-3.65	-3.03	0.62	B3LYP/6-31G (d, p)	[39]
56	-5.91	-6.17	0.26	-3.79	-3.71	0.08	B3LYP/6-31G*	[40]
57	-5.89	-6.11	0.22	-3.81	-3.68	0.13	B3LYP/6-31G*	[40]
58	-5.82	-5.75	0.07	-3.55	-3.54	0.01	B3LYP/6-31G+(d,p)	[41]
59	-4.79	-5.66	0.87	-3.57	-4.83	1.26	B3LYP/6-31+G(d,p)	[42]
60	-4.87	-5.76	0.89	-3.61	-4.88	1.27	B3LYP/6-31+G(d,p)	[42]
61	-4.92	-5.82	0.9	-3.63	-4.93	1.3	B3LYP/6-31+G(d,p)	[42]
62	-4.94	-5.88	0.94	-3.64	-4.99	1.35	B3LYP/6-31+G(d,p)	[42]
63	-5.07	-6	0.93	-3.74	-5.12	1.38	B3LYP/6-31+G(d,p)	[42]
64	-5.45	-5.04	0.41	-2.59	-1.9	0.69	B3LYP-6-31G(d,p)	[43]
65	-5.26	-4.9	0.36	-2.69	-2.05	0.65	B3LYP/6-31+G(d,p)	[43]
66	-5.1	-5.1	0	-2.3	-1.9	0.4	B3LYP/ 6-31G**	[44]
67	-5.24	-4.98	0.26	-2.82	-2.8	0.02	B3LYP/6-31G(d, p)	[45]
68	-5.04	-4.84	0.2	-2.7	-2.45	0.25	B3LYP/6-31G(d, p)	[45]
69	-5.3	-4.68	0.62	-3.18	-2.82	0.36	B3LYP/6-31G(d)	[46]
70	-5.3	-4.68	0.62	-3.2	-2.83	0.37	B3LYP/6-31G(d, p)	[46]
71	-5.57	-5.54	0.03	-3.94	-3.55	0.39	B3LYP/6-31G(d,p)	[47]
72	-5.59	-5.54	0.05	-3.89	-3.54	0.35	B3LYP/6-31G(d,p)	[47]
73	-5.67	-5.81	0.14	-3.94	-3.6	0.34	B3LYP/6-31G(d)	[48]
74	-5.62	-5.76	0.14	-3.92	-3.55	0.37	B3LYP/6-31G(d)	[48]
75	-5.58	-5.66	0.08	-3.85	-3.42	0.43	B3LYP/6-31G(d)	[48]
76	-5.31	-4.66	0.65	-3.24	-2.72	0.52	B3LYP/6-	[49]

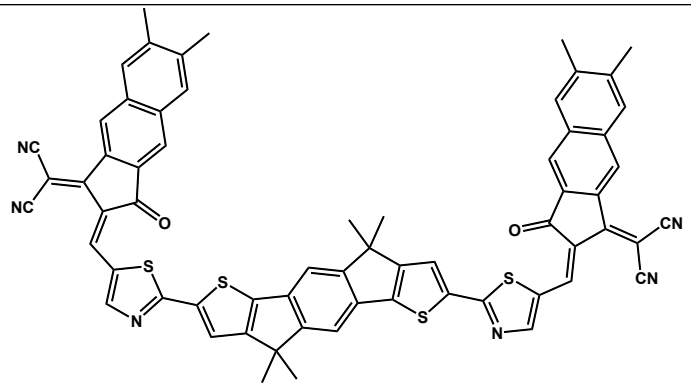
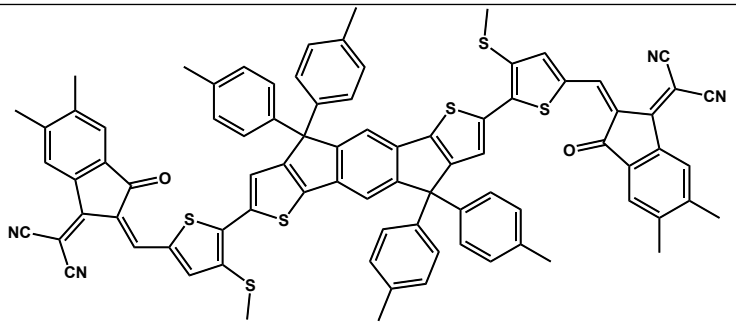
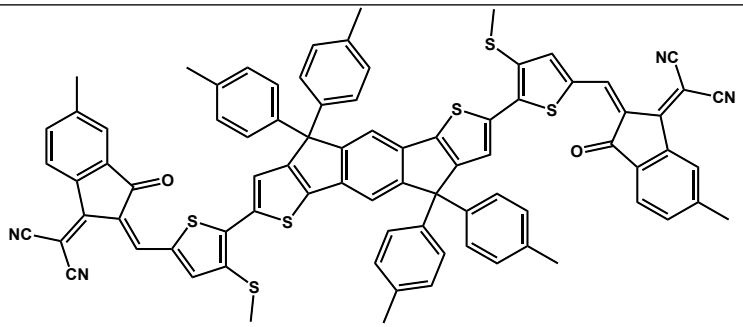
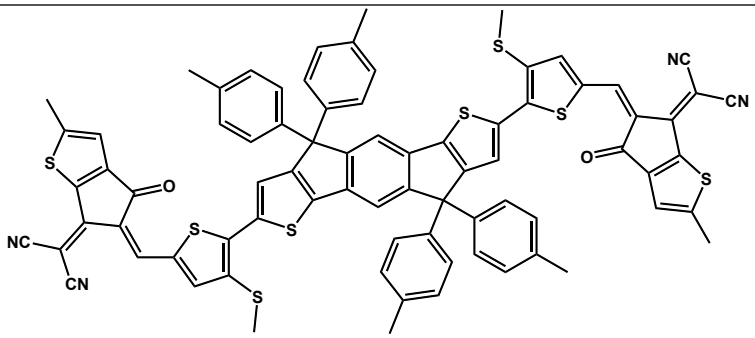
							31G(d)	
77	-5.48	-4.78	0.7	-3.32	-2.81	0.51	B3LYP/6-31G(d)	[49]
78	-5.33	-5.05	0.28	-3.27	-2.8	0.47	B3LYP/6-31G(d)	[49]
79	-5.84	-5.74	0.1	-4.06	-3.51	0.55	B3LYP/6-31G(d, p)	[50]
80	-5.75	-5.64	0.11	-4.04	-3.47	0.57	B3LYP/6-31G(d, p)	[50]
81	-5.69	-5.57	0.12	-4.01	-3.44	0.57	B3LYP/6-31G(d, p)	[50]
82	-5.45	-5.18	0.27	-3.79	-3.27	0.52	B3LYP/6-31G	[51]
83	-5.7	-5.8	0.1	-3.87	-3.29	0.58	B3LYP/6-31G(d)	[52]
84	-5.73	-5.95	0.22	-3.93	-5.95	2.02	B3LYP/6-31G(d)	[52]
85	-4.02	-6.03	2.01	-5.78	-3.58	2.2	B3LYP/6-31G(d)	[52]
86	-5.47	-5.25	0.22	-3.9	-3.29	0.61	B3LYP/6–31G**	[53]
87	-5.32	-5.06	0.26	-3.95	-3.3	0.65	B3LYP/6–31G**	[53]
88	-5.51	-5.45	0.06	-3.9	-3.39	0.51	B3LYP/6-31G(d)	[54]
89	-5.5	-5.37	0.13	-3.97	-3.35	0.62	B3LYP/6-31G(d)	[54]
90	-5.61	-5.47	0.14	-4.04	-3.41	0.63	B3LYP/6-31G(d)	[54]
91	-5.32	-5.35	0.03	-3.85	-3.36	0.49	B3LYP/6-31G(d)	[55]
92	-5.49	-5.53	0.04	-4.09	-3.59	0.5	B3LYP/6-31G(d)	[55]
93	-5.67	-5.58	0.09	-3.85	-3.42	0.43	B3LYP/6-31G(d,p)	[56]
94	-5.53	-5.64	0.11	-3.83	-3.56	0.27	B3LYP/6-31G	[57]
95	-5.5	-5.56	0.06	-3.81	-3.48	0.33	B3LYP/6-31G	[57]
96	-5.66	-5.7	0.04	-3.86	-3.6	0.26	B3LYP/6-31G	[57]
97	-5.99	-5.75	0.24	-3.95	-3.49	0.46	B3LYP/6-31G*	[58]
98	-5.74	-5.46	0.28	-3.93	-3.5	0.43	B3LYP/6-31G*	[58]
99	-5.62	-5.67	0.05	-3.9	-3.59	0.31	B3LYP/6-	[59]

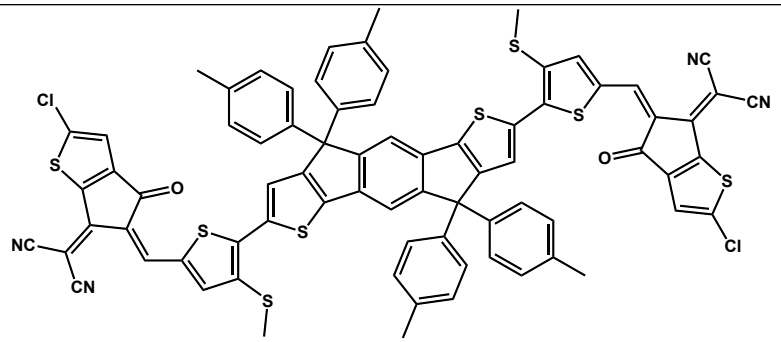
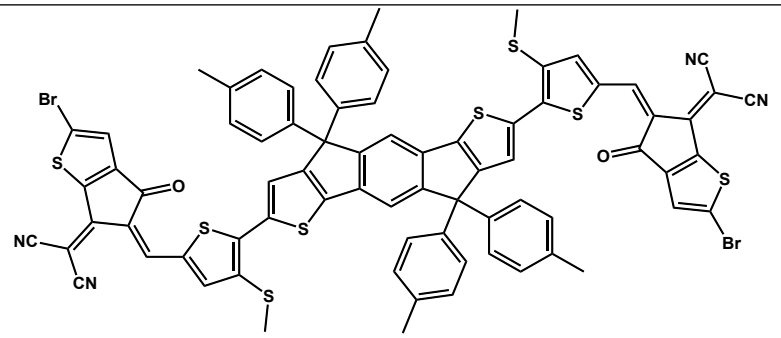
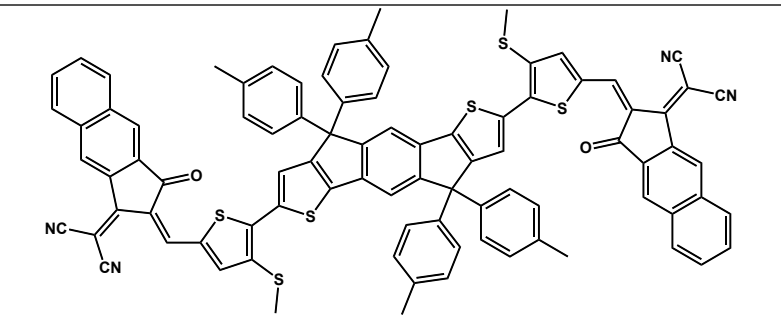
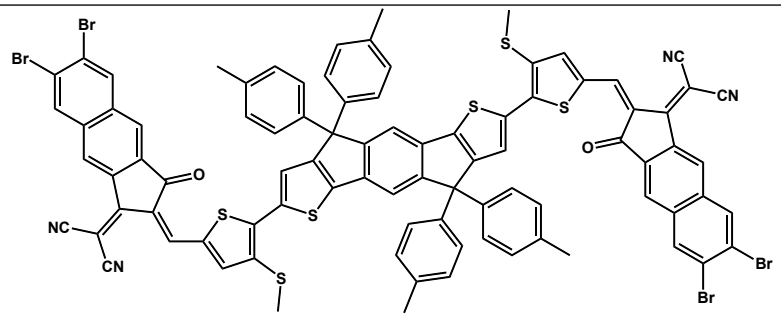
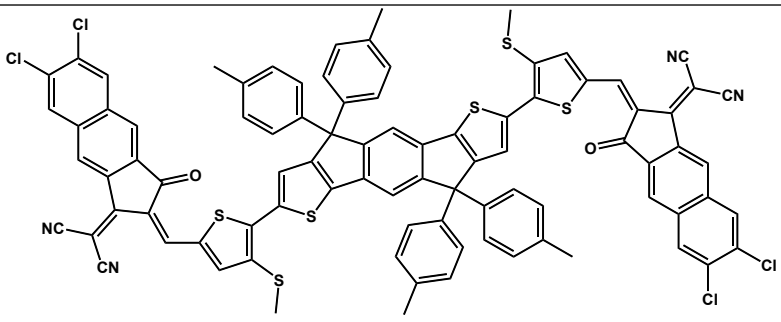
							31G(d,p)	
100	-5.54	-5.53	0.01	-3.91	-3.55	0.36	B3LYP/6-31G(d,p)	[59]
101	-5.6	-5.42	0.18	-3.65	-2.85	0.8	B3LYP/6-31G**	[60]
102	-5.57	-5.4	0.17	-3.63	-2.89	0.74	B3LYP/6-31G**	[60]
103	-5.75	-5.66	0.09	-3.7	-2.91	0.79	B3LYP/6-31G**	[60]
104	-5.48	-5.4	0.08	-3.35	-2.45	0.9	B3LYP/6-31G (d)	[61]
105	-5.39	-5.17	0.22	-2.84	-2.13	0.71	B3LYP/6-31G (d)	[61]
106	-5.81	-6.2	0.39	-3.95	-4.03	0.08	B3LYP/6-311G**	[62]
107	-5.6	-5.7	0.1	-3.95	-3.8	0.15	B3LYP/6-311G**	[62]
108	-5.62	-5.8	0.18	-3.57	-3.22	0.35	B3LYP/6-311+G(d,p)	[63]
109	-5.64	-6.2	0.56	-4.1	-4.21	0.11	B3LYP/6-311+G(d,p)	[63]
110	-5.75	-5.93	0.18	-3.56	-3.18	0.38	B3LYP/6-311+G(d,p)	[63]
111	-5.8	-6.37	0.57	-4.07	-4.06	0.01	B3LYP/6-311+G(d,p)	[63]
112	-5.3	-5.2	0.1	-3.6	-3.22	0.38	B3LYP/6-31G(d,p)	[64]
113	-5.6	-5.46	0.14	-3.6	-3.22	0.38	B3LYP/6-31G(d,p)	[64]
114	-5	-4.89	0.11	-3.6	-3.26	0.34	B3LYP/6-31G(d,p)	[64]
115	-5.95	-5.8	0.15	-4.02	-3.52	0.5	B3LYP/6-31G(d)	[65]
116	-6.01	-6.1	0.09	-3.8	-3.43	0.37	B3LYP/6-31G(d)	[65]
117	-5.98	-6.07	0.09	-3.77	-3.4	0.37	B3LYP/6-31G(d)	[65]
118	-5.96	-6.04	0.08	-3.76	-3.39	0.37	B3LYP/6-31G(d)	[65]
119	-6.34	-7.69	1.345	-3.73	-2.75	0.98	B3LYP/6-31G(d)	[66]
120	-6.38	-7.67	1.292	-3.98	-3.05	0.93	B3LYP/6-31G(d)	[66]
121	-5.87	-7.27	1.397	-3.9	-2.8	1.1	B3LYP/6-31G(d)	[67]
122	-6.05	-7.44	1.388	-3.89	-2.68	1.21	B3LYP/6-	[67]

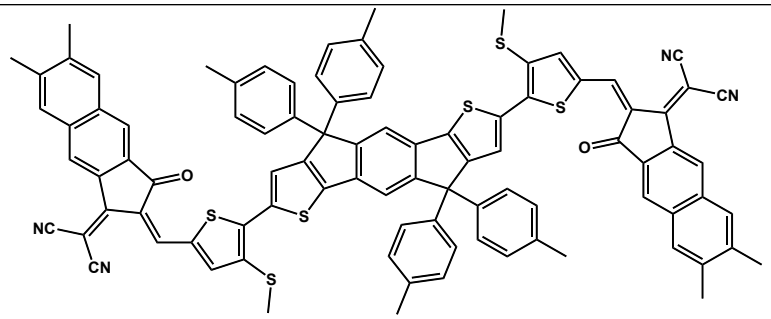
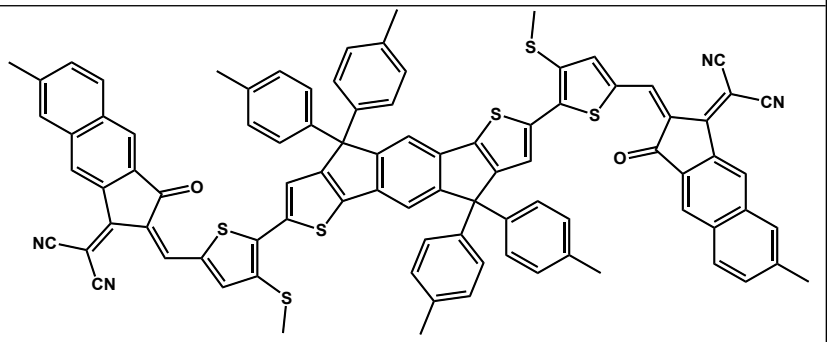
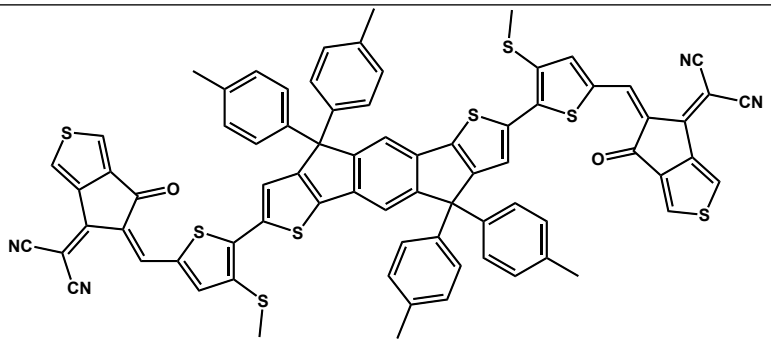
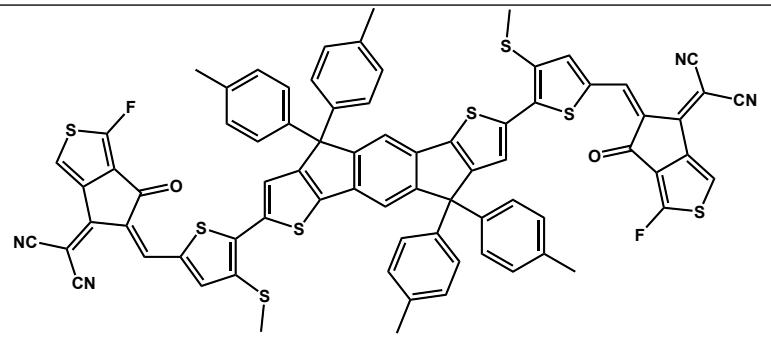
							31G(d)	
123	-5.8	-5.78	0.02	-3.9	-3.45	0.45	B3LYP/6-31G(d)	[68]
124	-6.1	-6.05	0.05	-4	-3.47	0.53	B3LYP/6-31G(d)	[68]
125	-5.4	-5.34	0.06	-3.8	-3.44	0.36	B3LYP/6-31G(d)	[69]
126	-5.82	-6.33	0.51	-3.49	-3.92	0.43	B3LYP/6-31G*	[70]
127	-5.97	-6.95	0.98	-4.11	-2.48	1.63	B3LYP/6-31G**	[71]
128	-5.73	-6.79	1.06	-4.18	-2.51	1.67	B3LYP/6-31G**	[71]
129	-5.95	-6.11	0.16	-3.57	-3.62	0.05	B3LYP/6-31G	[72]
130	-5.59	-5.54	0.05	-3.59	-3.49	0.1	B3LYP/6-31G	[72]

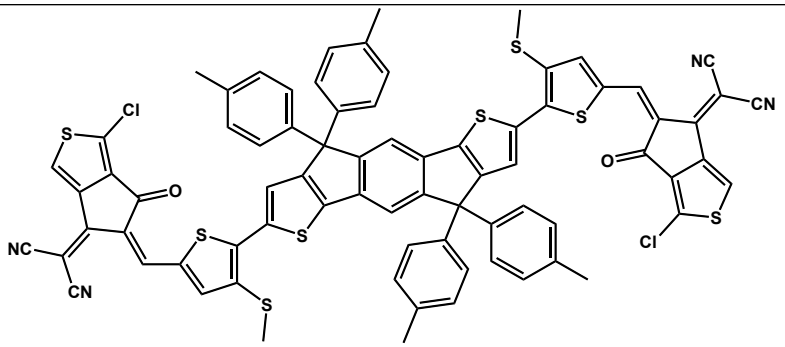
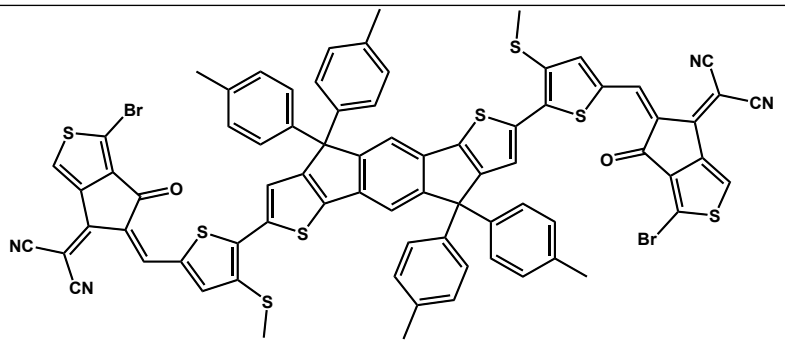
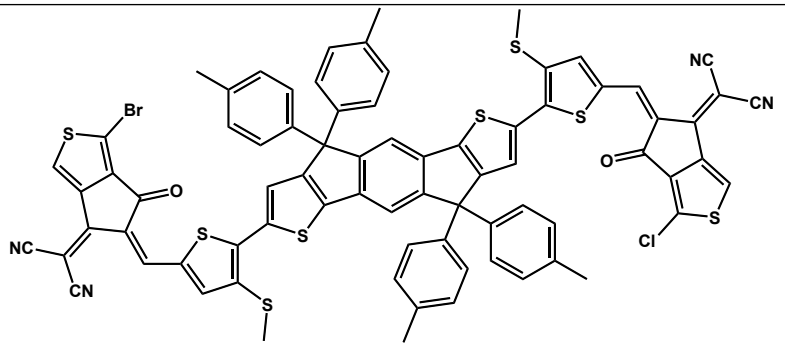
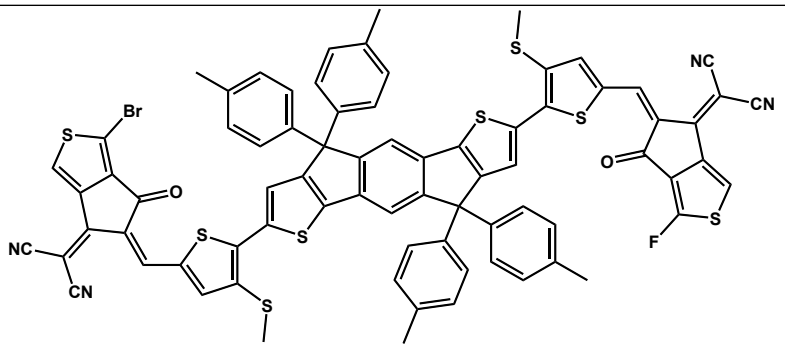
Table S3. HOMO energy level, LUMO energy level, PCE and structures of NFAs with >7.5% PCE for P3HT based OSCs

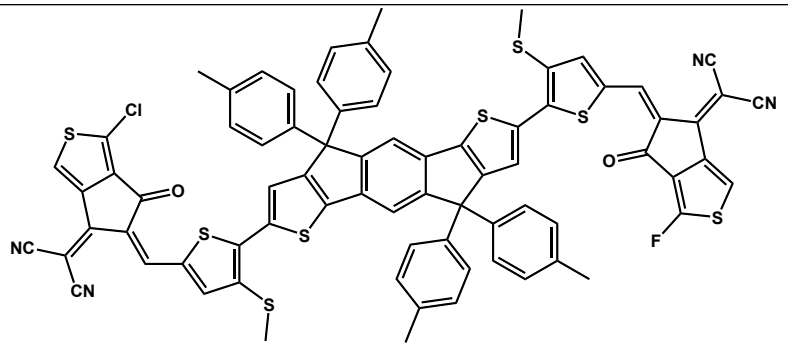
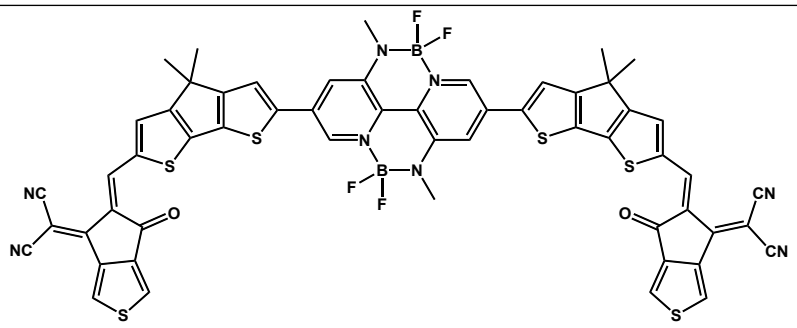
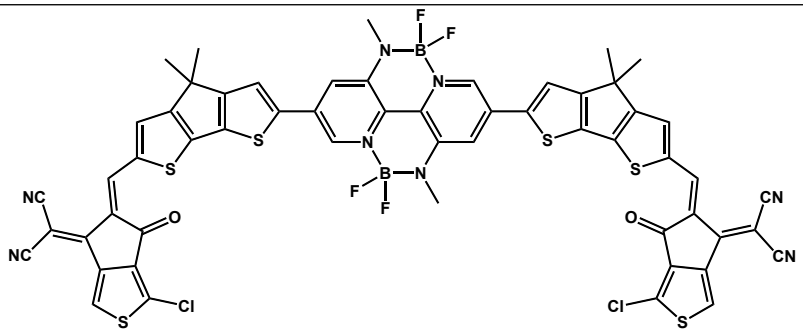
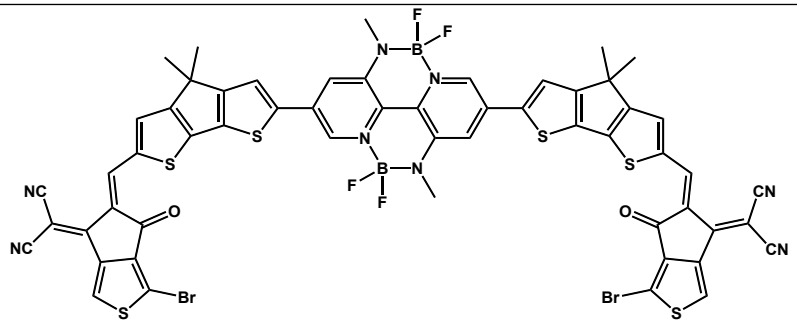
No	HOMO (eV)	LUMO (eV)	PCE (%)	Structure
1	5.368	3.726	8.101	
2	5.448	3.785	7.992	

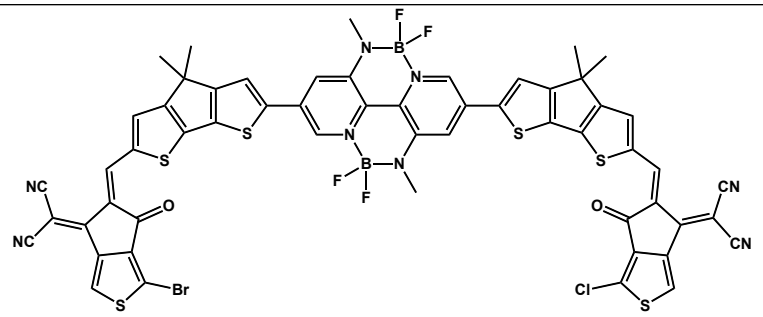
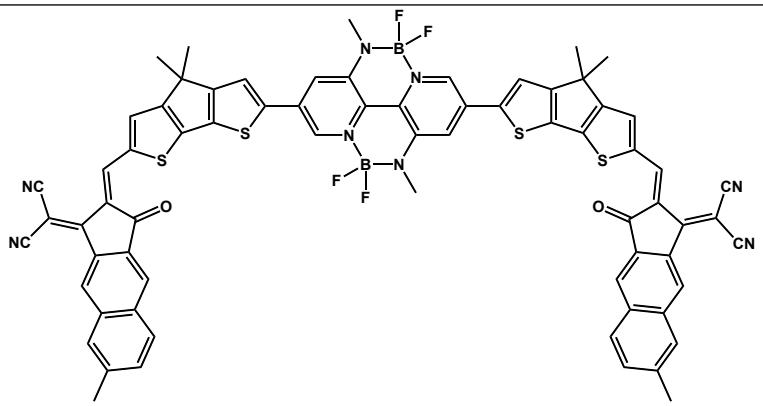
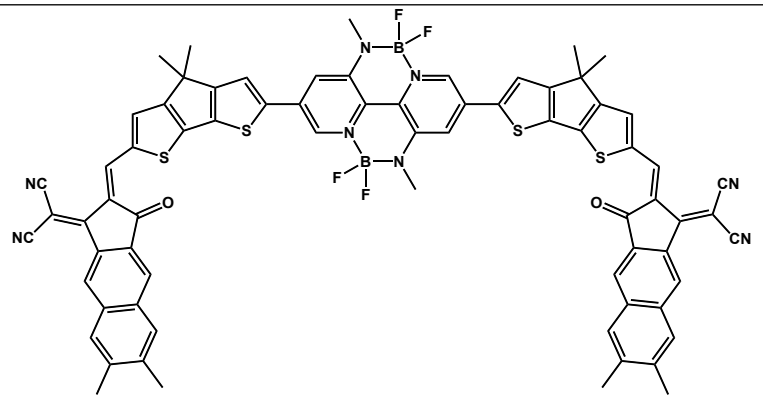
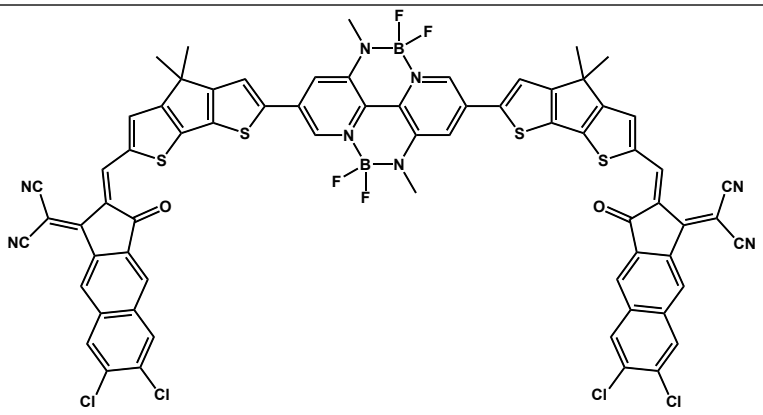
3	5.449	3.79	7.992	
4	5.41	3.694	7.888	
5	5.409	3.692	7.888	
6	5.373	3.758	7.58	

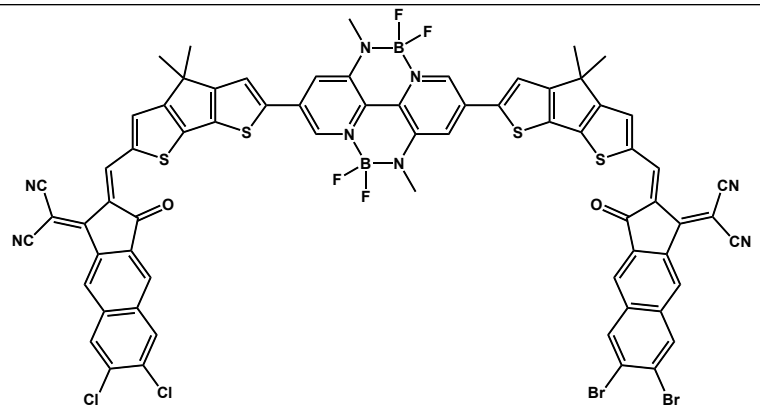
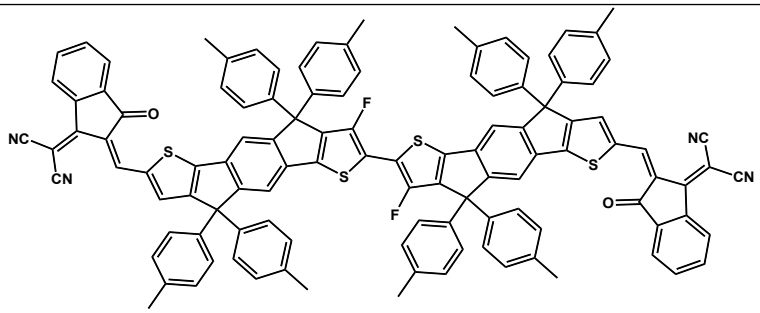
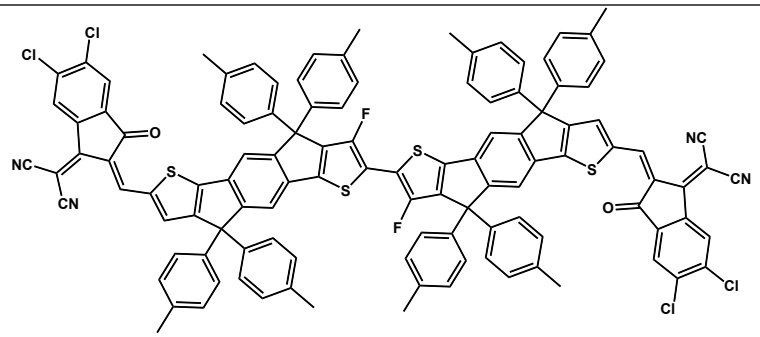
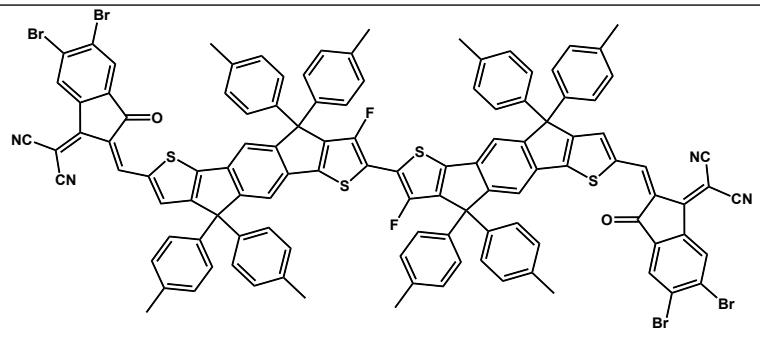
7	5.38	3.779	7.58	
8	5.379	3.773	7.58	
9	5.389	3.738	7.58	
10	5.392	3.752	7.58	
11	5.395	3.763	7.58	

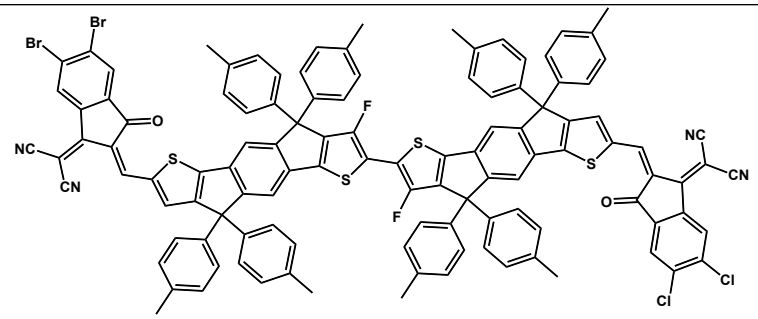
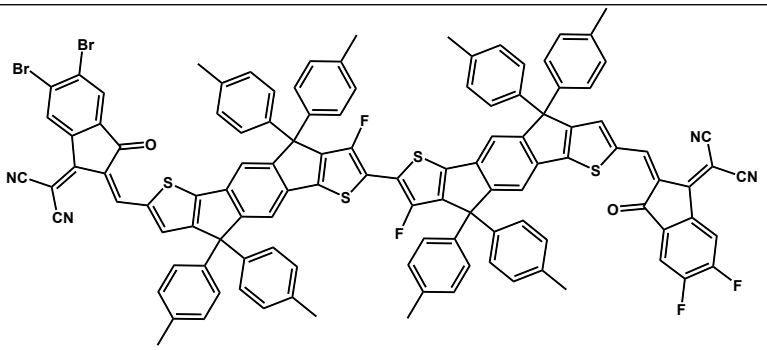
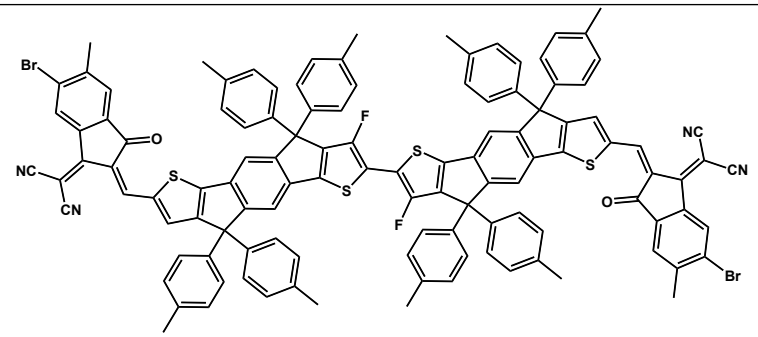
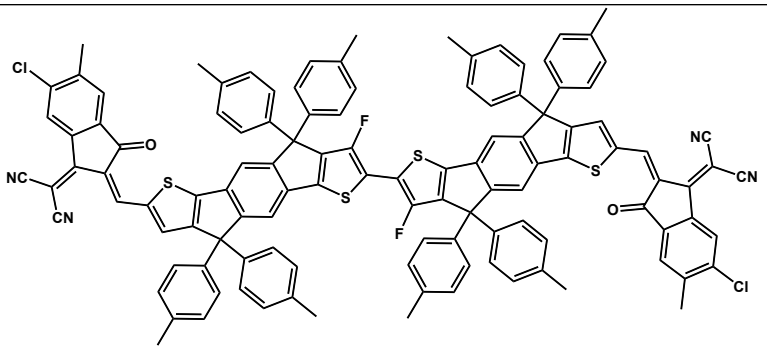
12	5.39	3.73	7.58	
13	5.388	3.73	7.58	
14	5.379	3.763	7.58	
15	5.401	3.794	7.58	

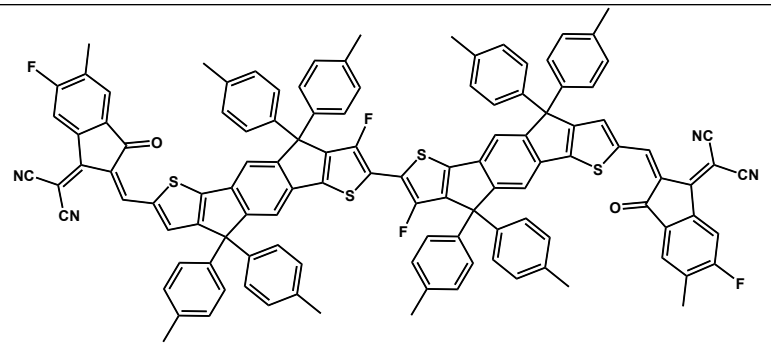
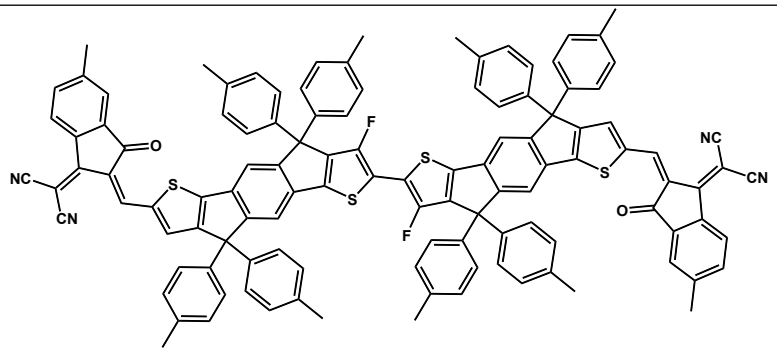
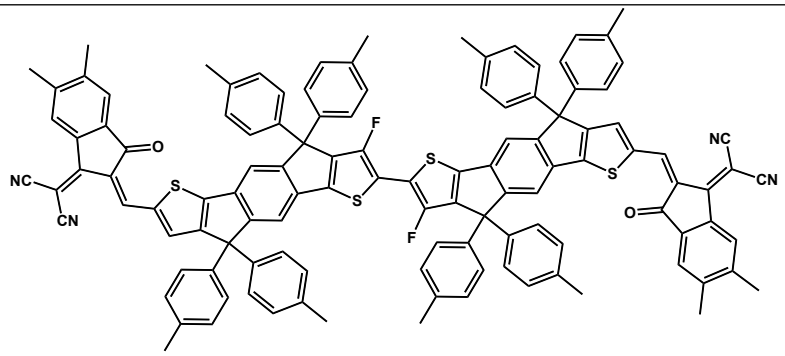
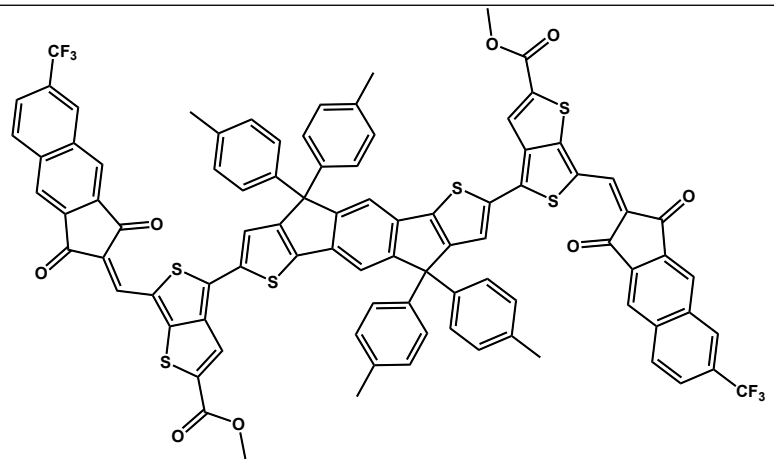
16	5.389	3.775	7.58	
17	5.385	3.77	7.58	
18	5.387	3.772	7.58	
19	5.393	3.784	7.58	

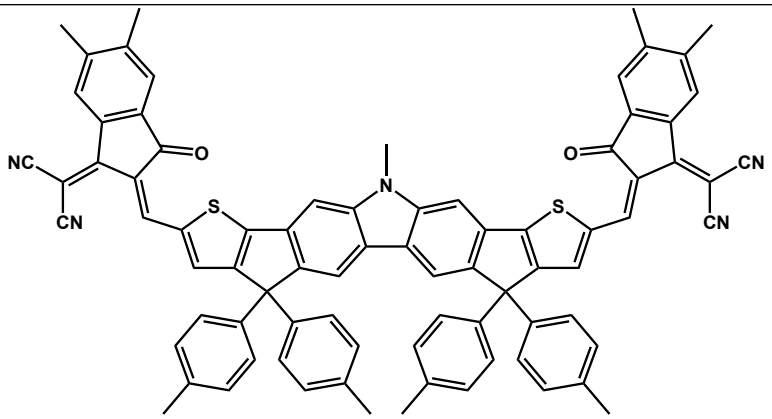
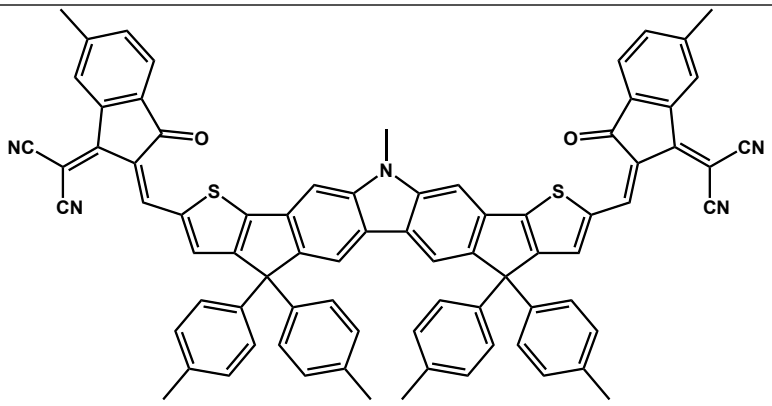
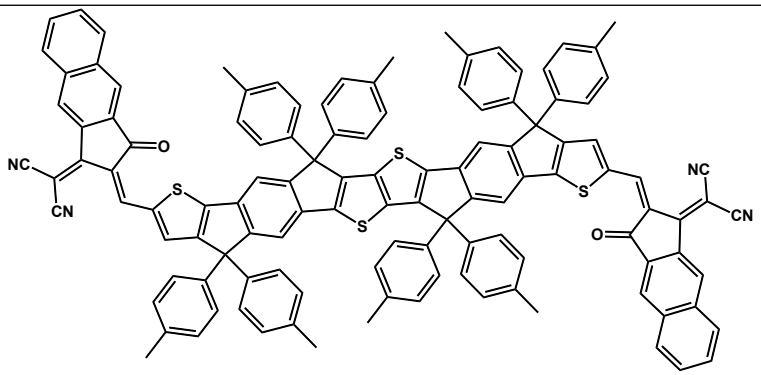
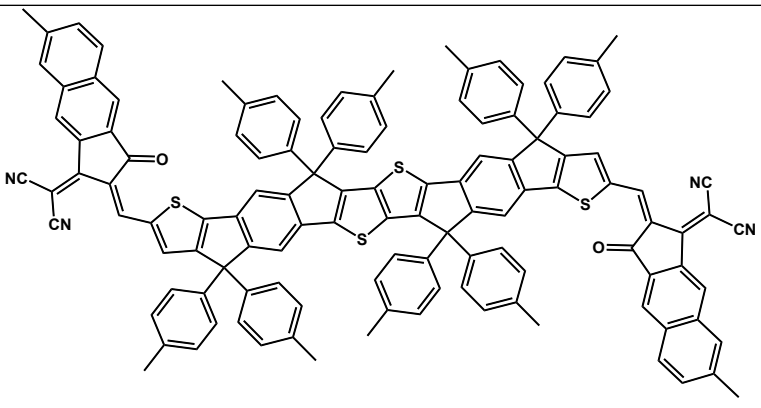
20	5.395	3.786	7.58	
21	5.45	3.79	7.52	
22	5.451	3.798	7.52	
23	5.451	3.798	7.52	

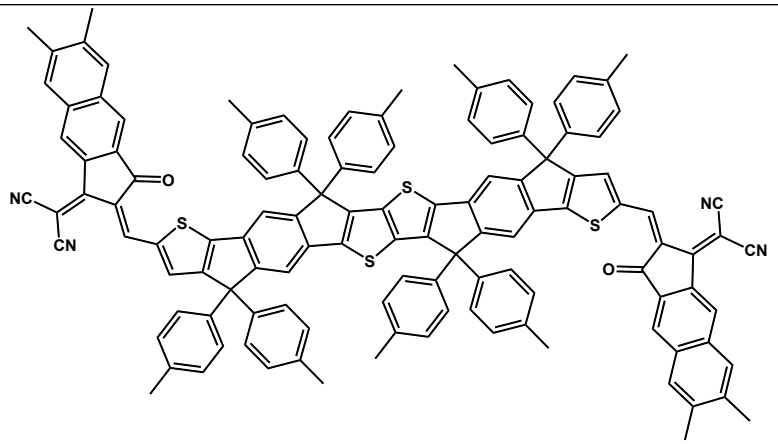
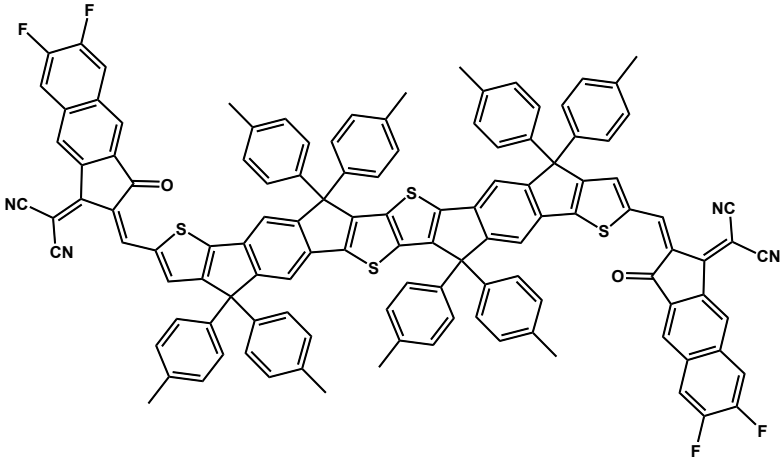
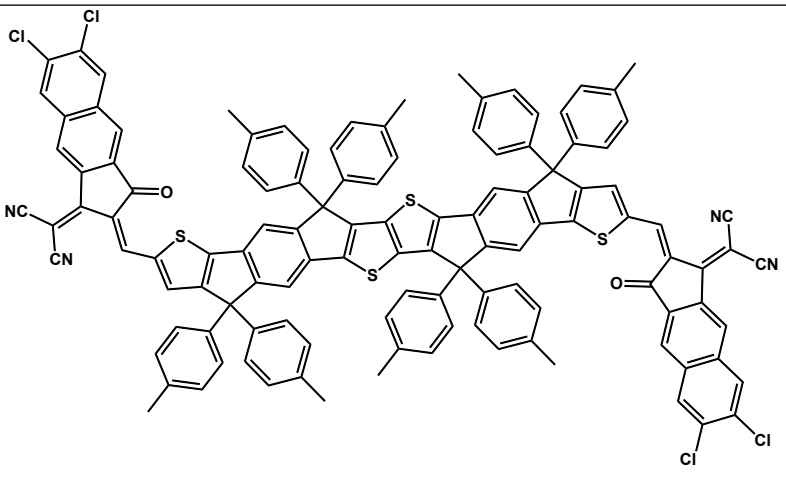
24	5.451	3.798	7.52	
25	5.497	3.77	7.52	
26	5.497	3.775	7.52	
27	5.462	3.785	7.52	

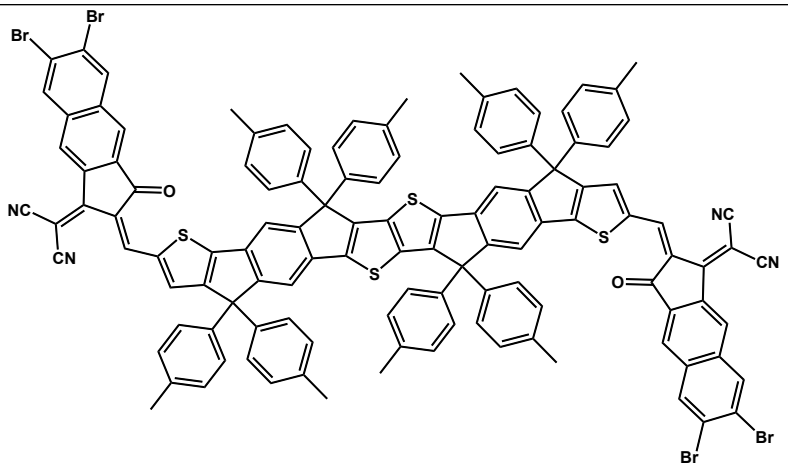
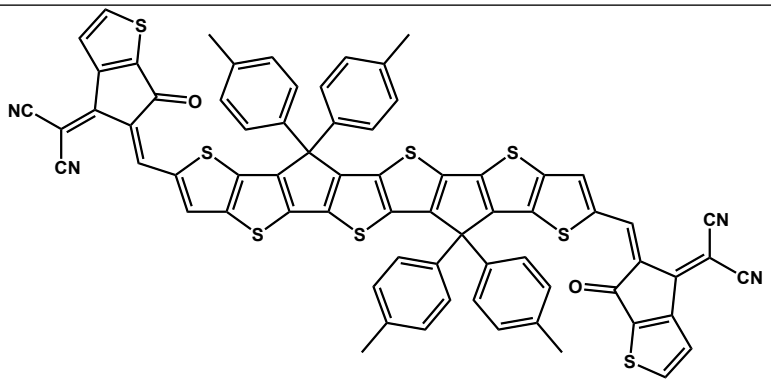
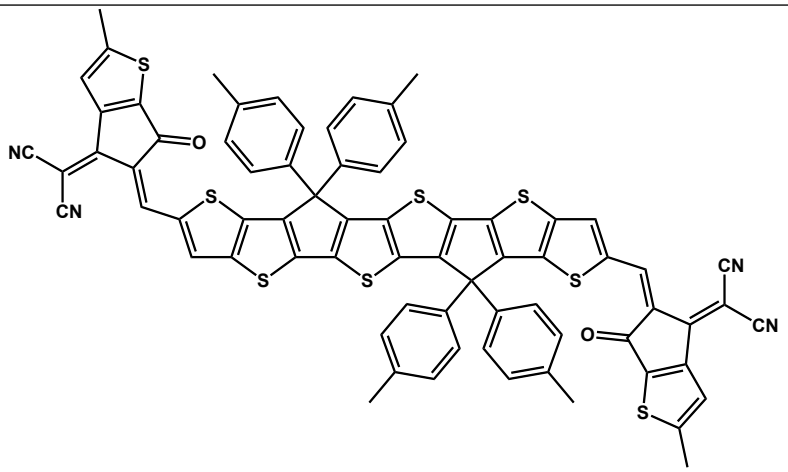
28	5.462	3.785	7.52	
29	5.401	3.679	7.58	
30	5.406	3.7	7.58	
31	5.403	3.69	7.58	

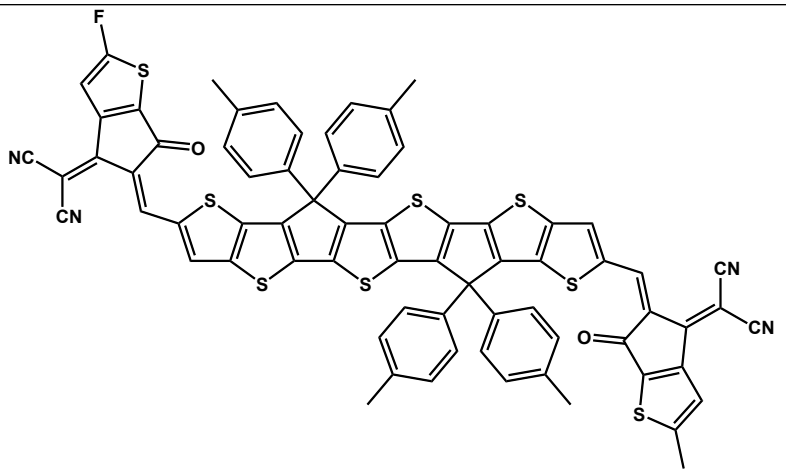
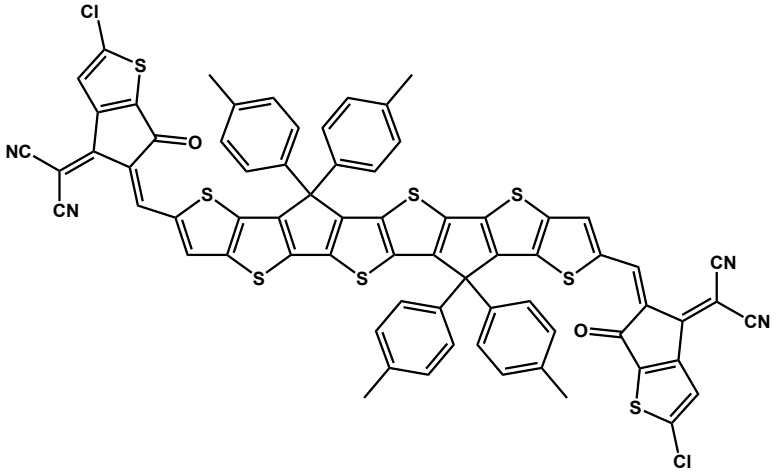
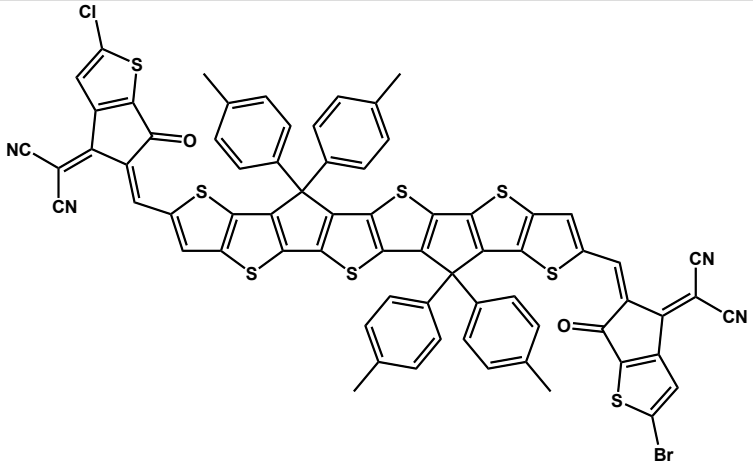
32	5.404	3.695	7.58	
33	5.409	3.742	7.58	
34	5.402	3.678	7.58	
35	5.405	3.682	7.58	

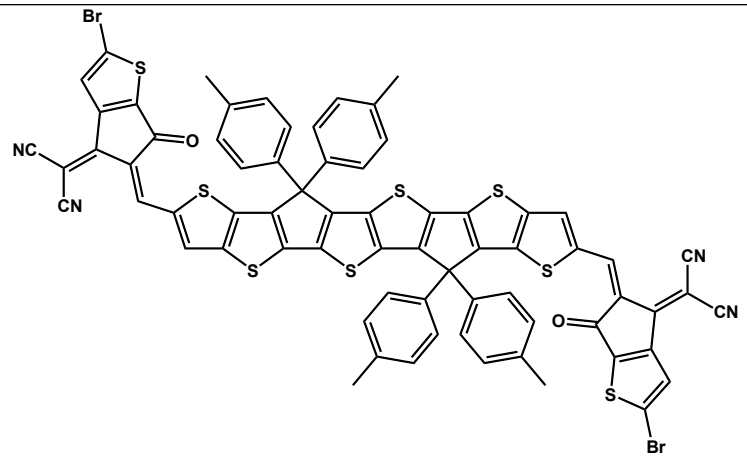
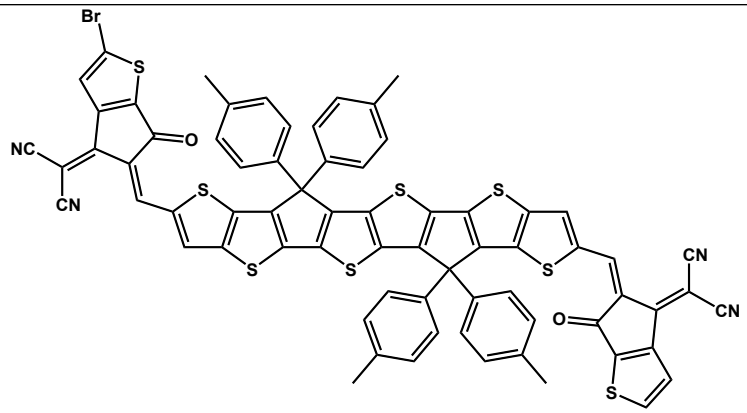
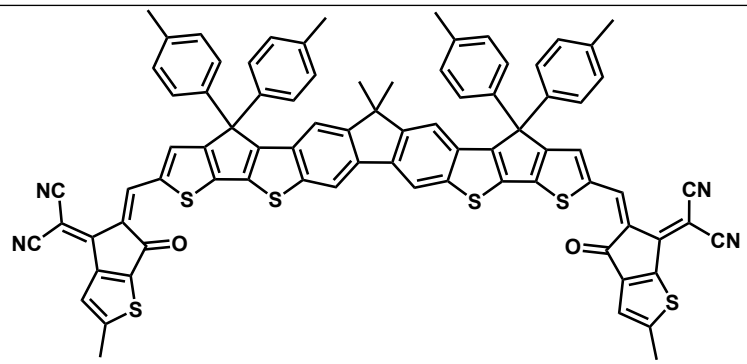
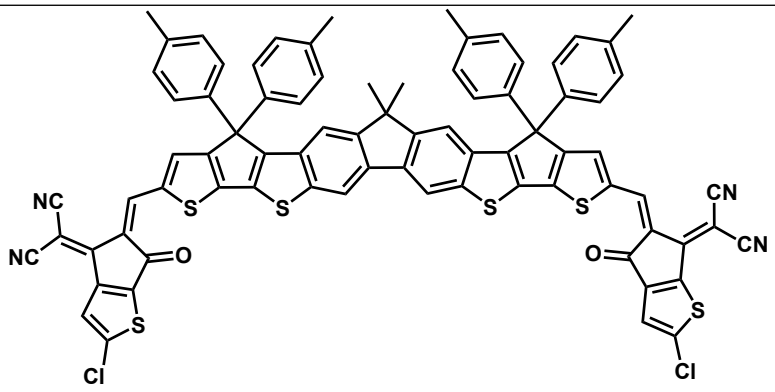
36	5.434	3.726	7.58	
37	5.399	3.673	7.58	
38	5.399	3.667	7.58	
39	5.5	3.768	7.964	

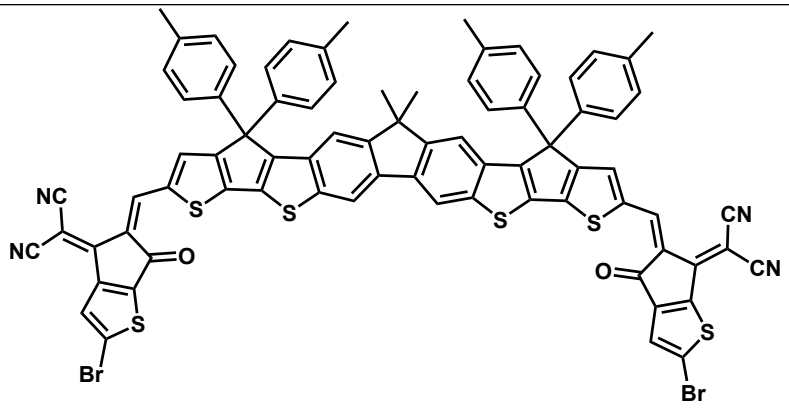
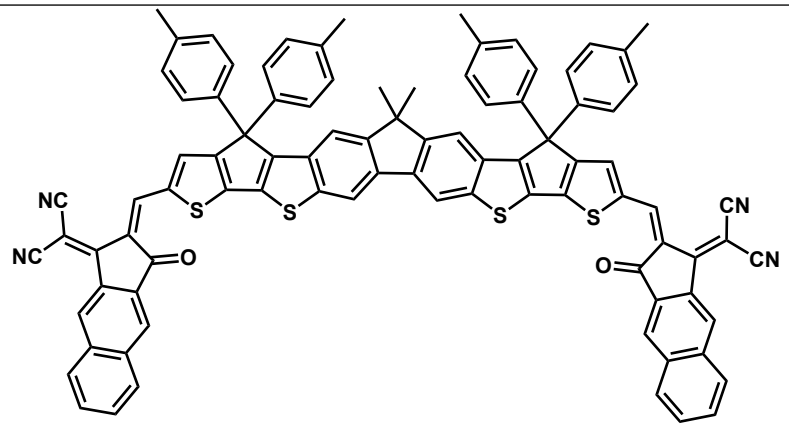
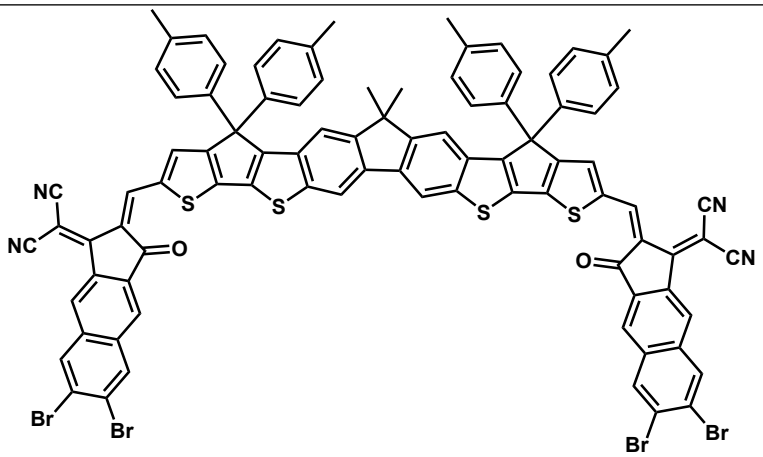
40	5.446	3.702	7.52	
41	5.445	3.708	7.52	
42	5.441	3.663	7.58	
43	5.44	3.654	7.58	

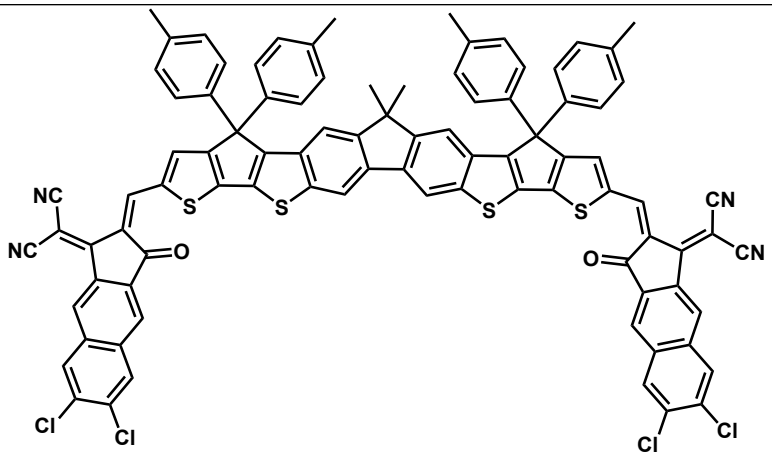
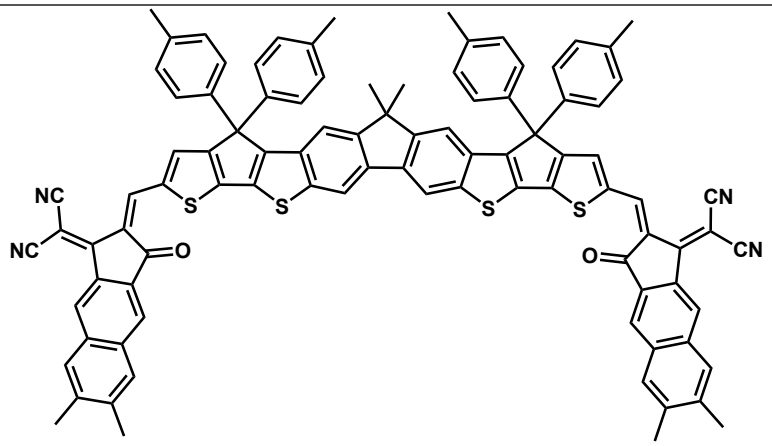
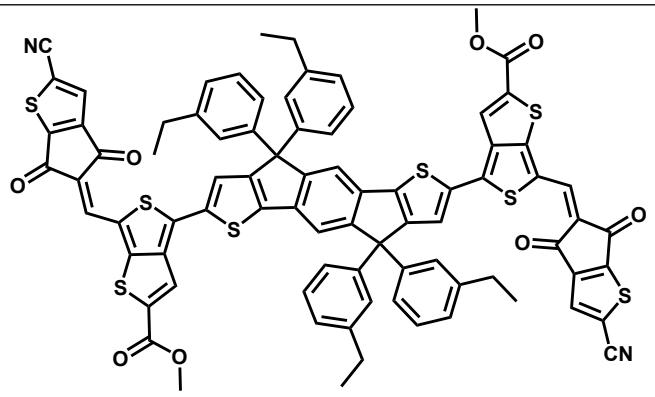
44	5.441	3.652	7.58	
45	5.476	3.754	7.58	
46	5.447	3.684	7.58	

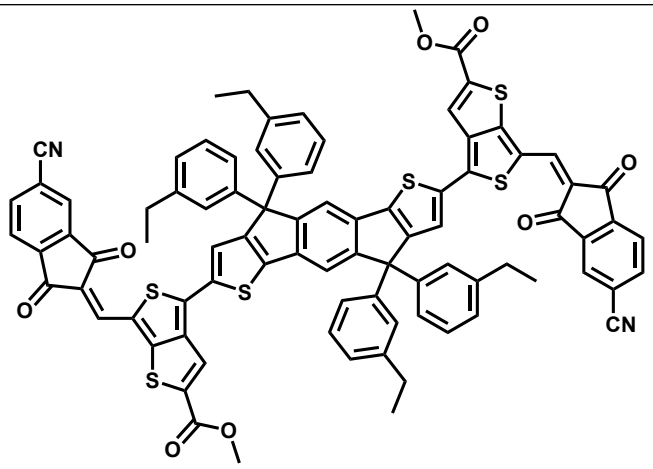
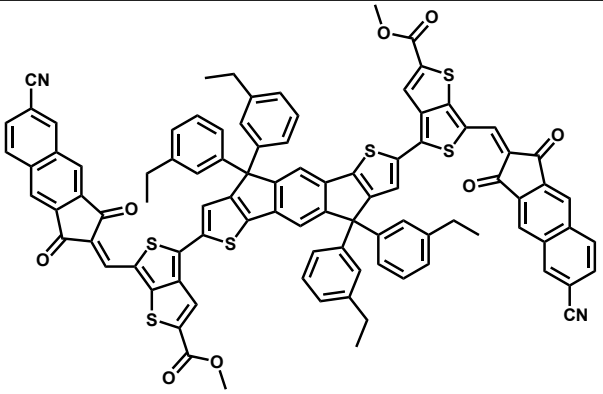
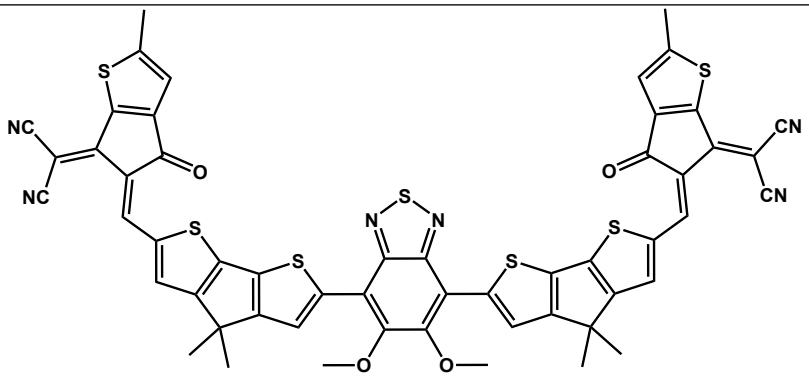
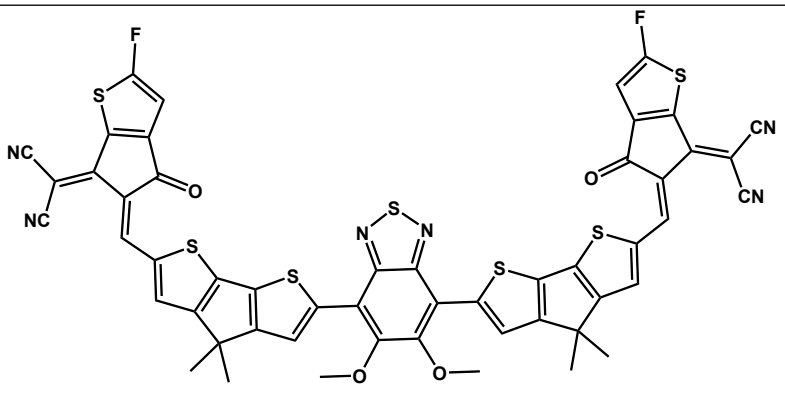
47	5.443	3.673	7.58	
48	5.444	3.755	7.52	
49	5.439	3.748	7.52	

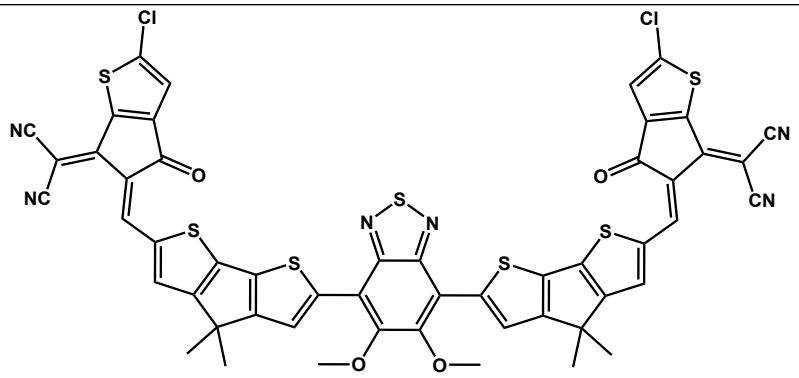
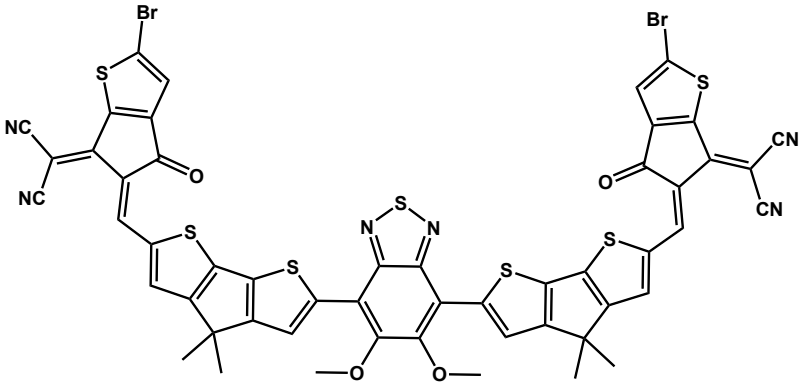
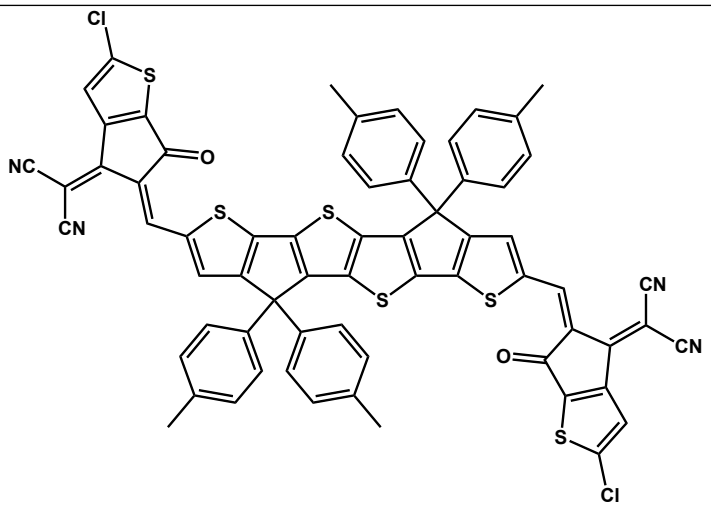
50	5.444	3.771	7.52	
51	5.445	3.769	7.52	
52	5.445	3.765	7.52	

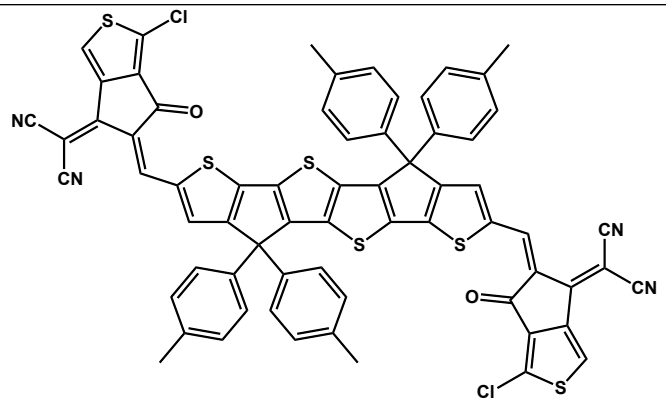
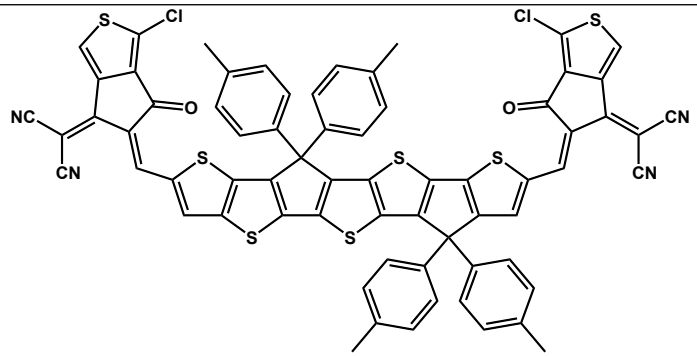
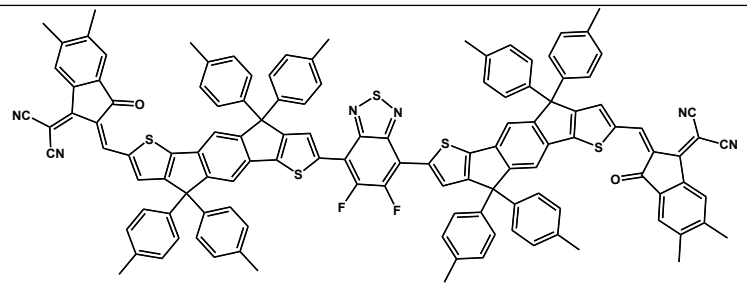
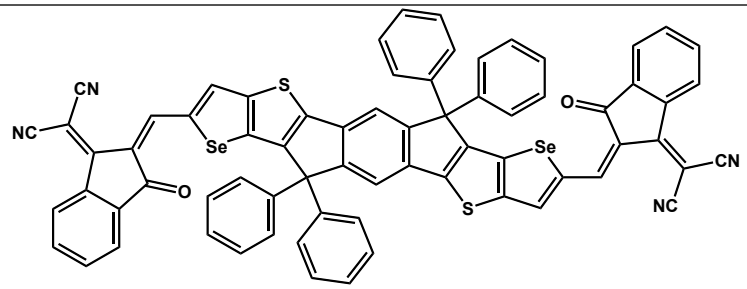
53	5.444	3.762	7.52	
54	5.444	3.759	7.52	
55	5.441	3.718	7.52	
56	5.455	3.756	7.52	

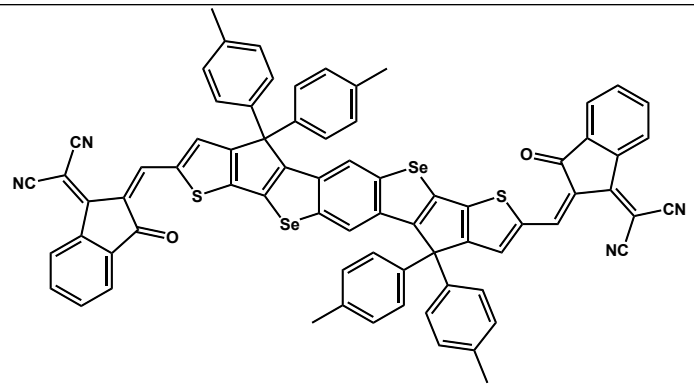
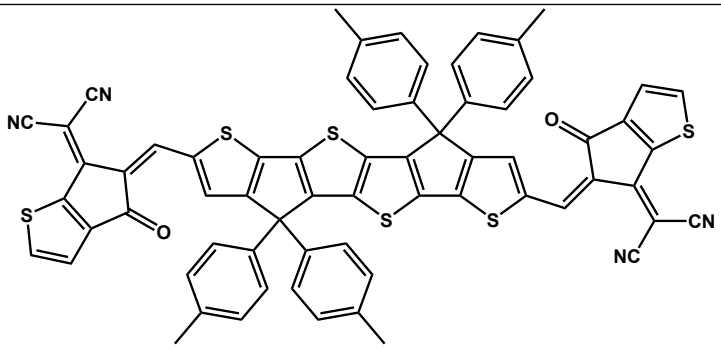
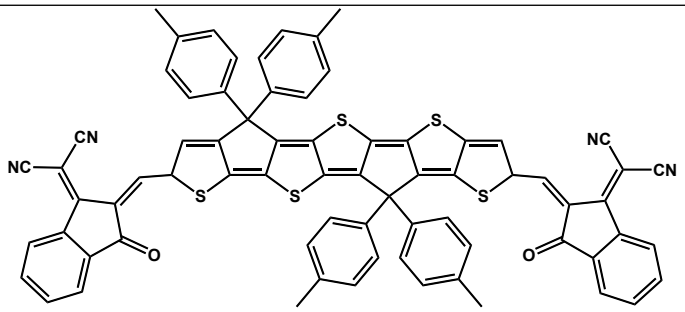
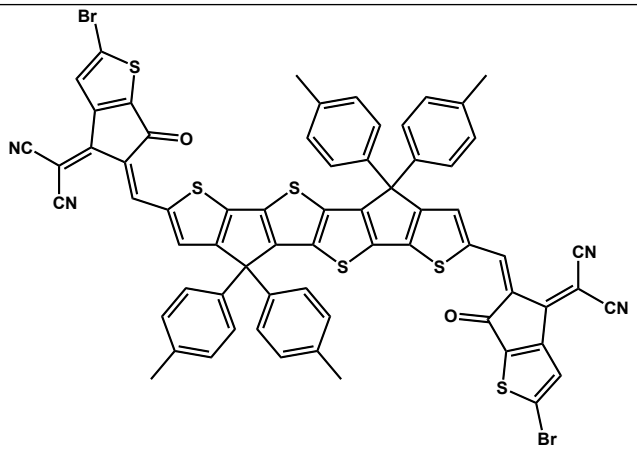
57	5.453	3.744	7.52	
58	5.45	3.706	7.52	
59	5.454	3.719	7.52	

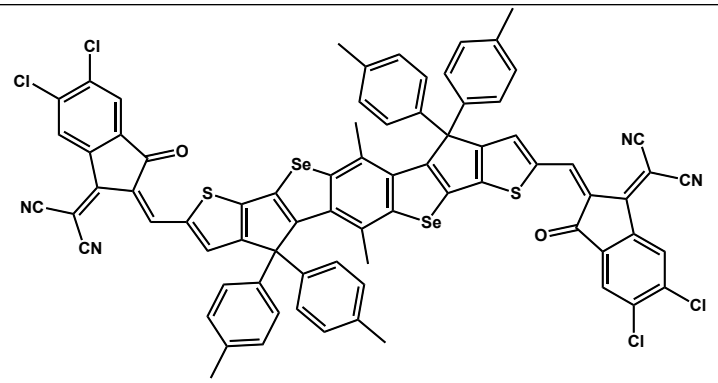
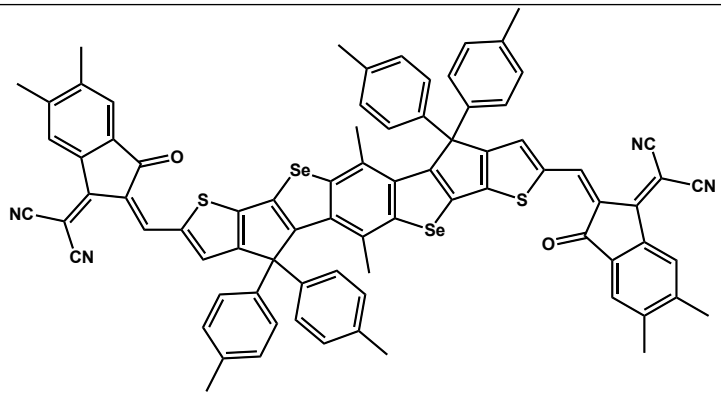
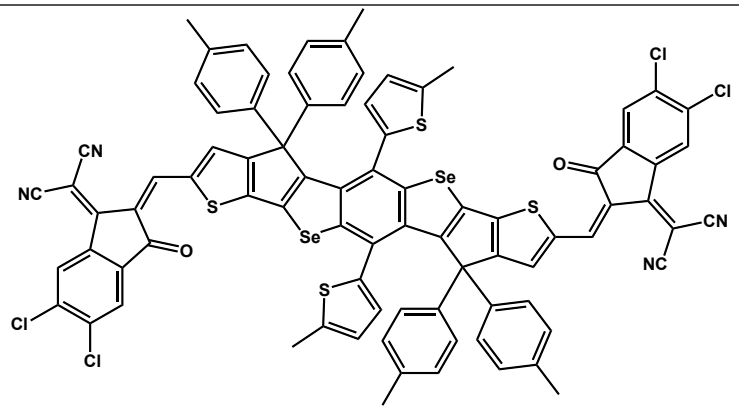
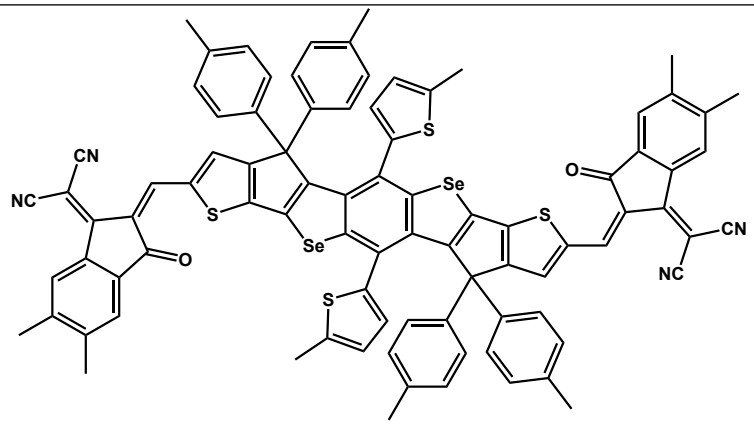
60	5.459	3.738	7.52	
61	5.449	3.684	7.52	
62	5.414	3.778	7.656	

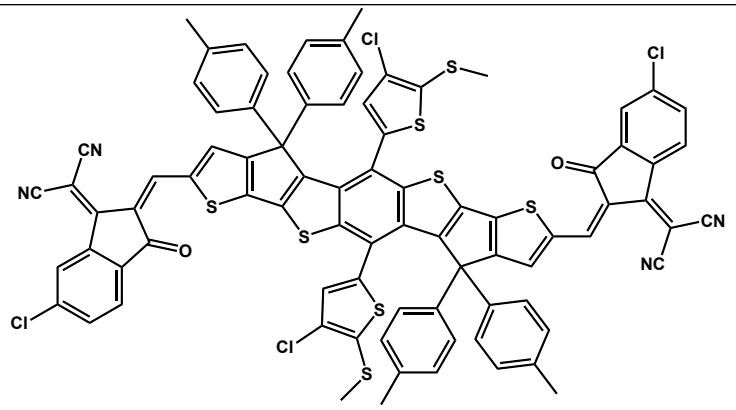
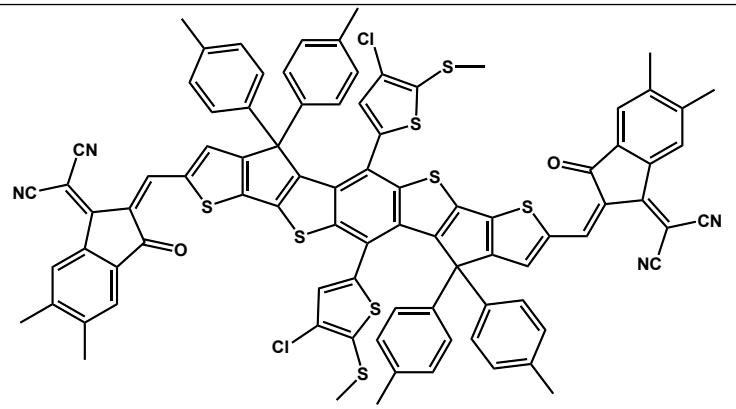
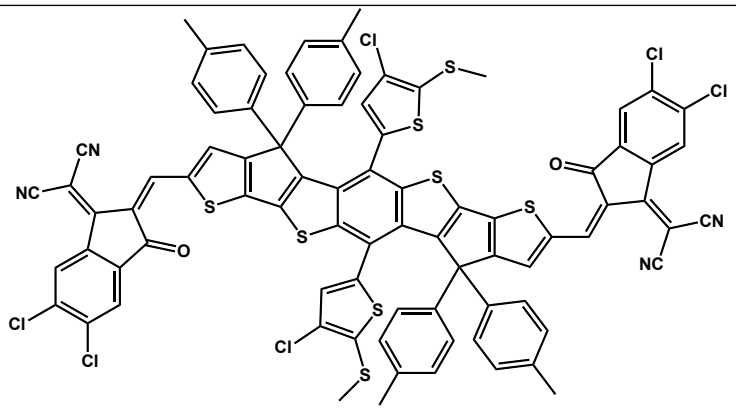
63	5.42	3.754	7.656	
64	5.426	3.749	7.656	
65	5.441	3.748	7.52	
66	5.441	3.754	7.52	

67	5.441	3.75	7.52	
68	5.441	3.75	7.52	
69	5.413	3.757	7.52	

70	5.431	3.761	7.52	
71	5.447	3.765	7.52	
72	5.422	3.696	7.888	
73	5.43	3.772	7.52	

74	5.424	3.72	7.52	
75	5.422	3.771	7.52	
76	5.43	3.796	7.888	
77	5.412	3.748	7.52	

78	5.435	3.75	7.52	
79	5.424	3.701	7.52	
80	5.419	3.726	7.52	
81	5.41	3.68	7.52	

82	5.451	3.714	8.284	
83	5.451	3.715	8.284	
84	5.451	3.724	8.284	

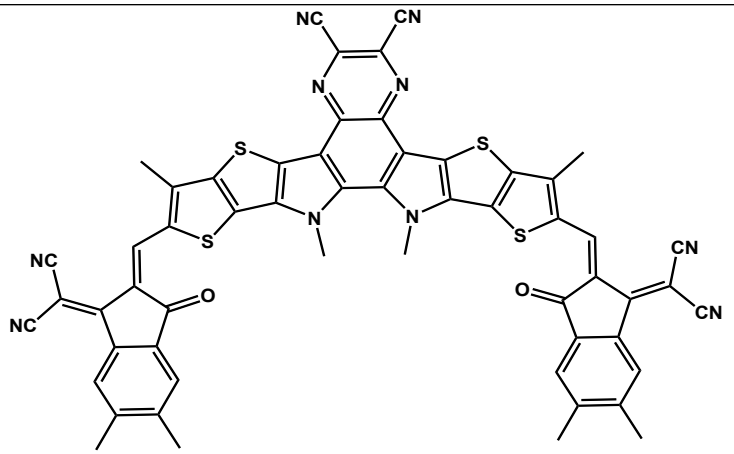
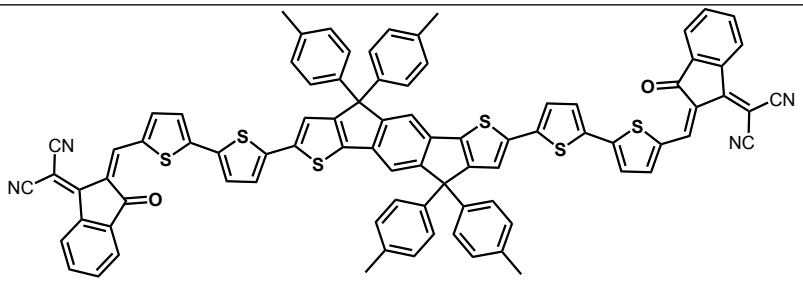
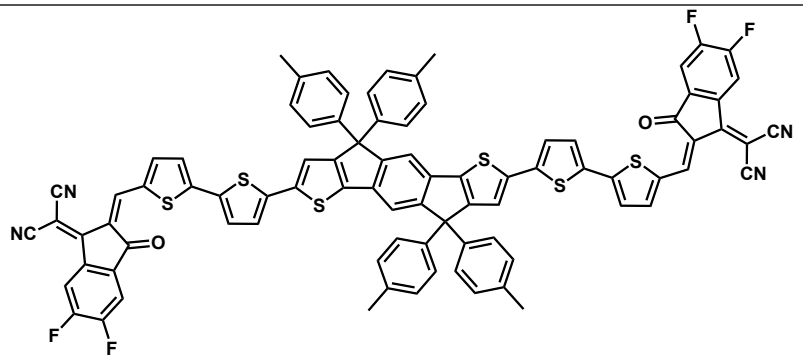
85	5.518	3.798	7.52	
86	5.357	3.694	7.52	
87	5.374	3.793	7.52	

Table S4. Green solvents for selected for 87 NFAs.

NFAs	Solvent 1	Solvent 2	Solvent 3	Solvent 4	Solvent 5
1	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
2	Ethyl Lactate	2-Butanol	1-Pentanol	1-Butanol	Acetone
3	1-Pentanol	Ethyl Lactate	Acetone	Butyl Lactate	1-Butanol
4	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
5	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
6	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
7	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
8	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
9	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
10	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole

11	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
12	Anisole	Ethyl Acetate	Acetone	2-Methylanisole	1-Pentanol
13	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
14	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
15	Acetone	Butyl Lactate	1-Pentanol	Anisole	2-Methylanisole
16	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
17	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
18	Acetone	Butyl Lactate	1-Pentanol	2-Butanol	Anisole
19	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
20	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
21	2-Butanol	Ethyl Lactate	1-Pentanol	1-Butanol	Acetone
22	1-Butanol	2-Butanol	Ethyl Lactate	1-Pentanol	Acetone
23	2-Butanol	Ethyl Lactate	1-Pentanol	1-Butanol	Acetone
24	2-Butanol	Ethyl Lactate	1-Pentanol	1-Butanol	Acetone
25	1-Butanol	Ethyl Lactate	2-Butanol	1-Pentanol	Acetone
26	Acetone	Butyl Lactate	1-Pentanol	2-Butanol	Anisole
27	1-Butanol	2-Butanol	Ethyl Lactate	1-Pentanol	Acetone
28	2-Butanol	Ethyl Lactate	1-Pentanol	1-Butanol	Acetone
29	Acetone	Butyl Lactate	1-Pentanol	2-Butanol	Anisole
30	Butyl Lactate	Acetone	Anisole	Ethyl Acetate	2-Methylanisole
31	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
32	Anisole	Ethyl Acetate	Butyl Lactate	2-Methylanisole	Acetone
33	Butyl Lactate	Acetone	Anisole	Ethyl Acetate	2-Methylanisole
34	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
35	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
36	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
37	Acetone	Butyl Lactate	1-Pentanol	2-Butanol	Anisole
38	Acetone	Butyl Lactate	1-Pentanol	2-Butanol	Anisole
39	1-Pentanol	Ethyl Lactate	Acetone	Butyl Lactate	1-Butanol
40	Acetone	Butyl Lactate	1-Pentanol	2-Butanol	Anisole
41	Acetone	Butyl Lactate	1-Pentanol	2-Butanol	Anisole
42	Acetone	Butyl Lactate	1-Pentanol	2-Butanol	Anisole
43	Acetone	Butyl Lactate	1-Pentanol	2-Butanol	Anisole
44	Acetone	Butyl Lactate	1-Pentanol	2-Butanol	Anisole
45	1-Pentanol	Ethyl Lactate	Acetone	Butyl Lactate	1-Butanol
46	1-Pentanol	Ethyl Lactate	Acetone	Butyl Lactate	1-Butanol
47	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
48	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
49	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
50	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
51	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
52	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
53	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
54	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
55	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole

56	Anisole	Ethyl Acetate	Butyl Lactate	2-Methylanisole	Acetone
57	Butyl Lactate	Acetone	Anisole	Ethyl Acetate	2-Methylanisole
58	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
59	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
60	Butyl Lactate	Acetone	Anisole	Ethyl Acetate	2-Methylanisole
61	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
62	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
63	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
64	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
65	1-Pentanol	2-Butanol	Ethyl Lactate	1-Butanol	Acetone
66	1-Butanol	Ethyl Lactate	2-Butanol	1-Pentanol	Acetone
67	1-Butanol	Ethyl Lactate	2-Butanol	1-Pentanol	Acetone
68	1-Butanol	Ethyl Lactate	2-Butanol	1-Pentanol	Acetone
69	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
70	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
71	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
72	Acetone	Butyl Lactate	1-Pentanol	2-Butanol	Anisole
73	Anisole	Ethyl Acetate	2-Methylanisole	Butyl Lactate	Acetone
74	Anisole	Ethyl Acetate	2-Methylanisole	Butyl Lactate	Acetone
75	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
76	Butyl Lactate	Acetone	Anisole	Ethyl Acetate	2-Methylanisole
77	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
78	Ethyl Acetate	Anisole	2-Methylanisole	Butyl Lactate	Acetone
79	Anisole	Ethyl Acetate	Butyl Lactate	2-Methylanisole	Acetone
80	Ethyl Acetate	Anisole	2-Methylanisole	Butyl Lactate	Acetone
81	Anisole	Ethyl Acetate	2-Methylanisole	Butyl Lactate	Acetone
82	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
83	Butyl Lactate	Acetone	Anisole	Ethyl Acetate	2-Methylanisole
84	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
85	1-Pentanol	Ethyl Lactate	Acetone	Butyl Lactate	1-Butanol
86	Butyl Lactate	Acetone	1-Pentanol	Ethyl Acetate	Anisole
87	Acetone	Butyl Lactate	1-Pentanol	2-Butanol	Anisole

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