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Informações Suplementares

Modelagem da Energia de Gibbs de Injeção de Elétrons de Corantes D-π-A Baseados em Trifenilaminas

Modeling the Gibbs Energy of Electron Injection of D-π-A dyes Based on Triphenylamines

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1. Multicolinearidade e Significância dos Descritores

Para o teste de multicolinearidade - quão correlacionada uma variável está com -, uma métrica comumente empregada é o VIF (do inglês *"Variance inflation factor"*), dada pela Eq. S1. Basicamente, o VIF de um dado descritor *i* é calculado a partir do o coeficiente de determinação R^2 de uma regressão utilizando *i* como variável dependente e o restante dos descritores como variável independente. Assim podemos dizer o quão correlacionado com os outros descritores *i* está: não correlacionado, $VIF_i = 1$; ii) moderadamente correlacionado, $1 < VIF_i \leq 5$ ou; iii) fortemente correlacionado, $VIF_i > 5$. Sendo que valores entre $1 < VIF_i \leq 5$ podem ser considerados satisfatórios.

$$VIF_i = \frac{1}{1-R_i^2} \quad \textbf{(S1)}$$

A partir dos valores de VIF dispostos na Tabela S1, podemos afirmar que os descritores estão moderadamente correlacionados, satisfazendo o critério de multicolinearidade.

Tabela S1. Significância estatística e fator da inflação de variância (VIF) dos descritores dos modelos obtidos: M-1 e M-2.

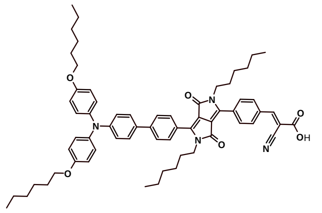
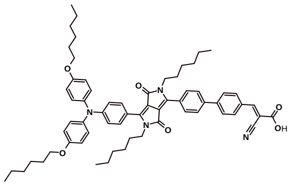
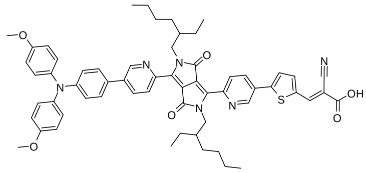
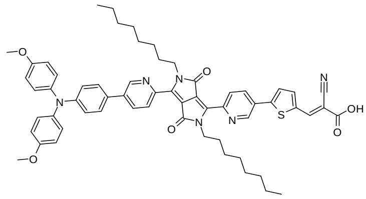
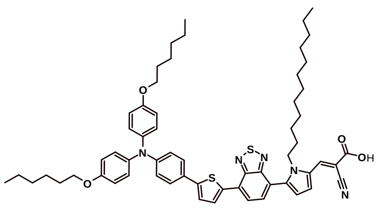
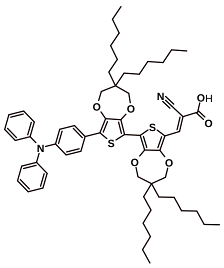
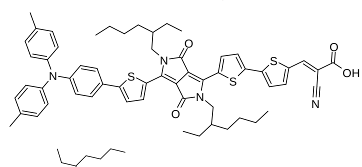
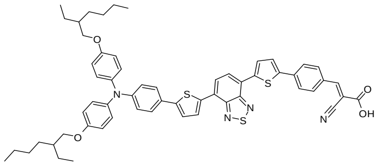
M-1	**Valor-p**	**VIF**	**M-2**	**Valor-p**	**VIF**
Eletroafinidade	$2{,}00\cdot10^{-16}$	1,622	Eletroafinidade	$2{,}00\cdot10^{-16}$	1,556
minsssN	$7{,}49\cdot10^{-5}$	3,894	minsssN	$1{,}45\cdot10^{-6}$	4,691
nT10Ring	$7{,}31\cdot10^{-9}$	2,912	nT10Ring	$2{,}37\cdot10^{-7}$	1,497
GATS8s	$3{,}65\cdot10^{-3}$	1,494	GATS8s	$1{,}11\cdot10^{-4}$	1,490
nRing	$1{,}29\cdot10^{-6}$	4,579	MDEN_23	$2{,}62\cdot10^{-7}$	4,794
nHeteroRing	$1{,}10\cdot10^{-8}$	4,628	MLFER_BO	$6{,}50\cdot10^{-3}$	4,162
nT10HeteroRing	$2{,}36\cdot10^{-3}$	1,435	MLFER_S	$9{,}34\cdot10^{-8}$	3,685
-	-	-	nS	$2{,}51\cdot10^{-3}$	1,692
-	-	-	RDF30m	$1{,}32\cdot10^{-3}$	1,820

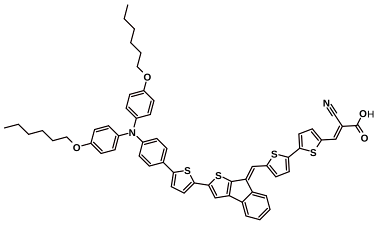
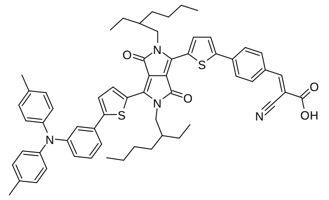
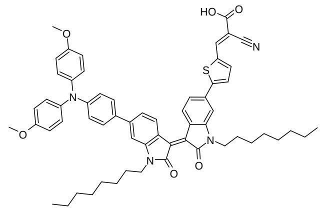
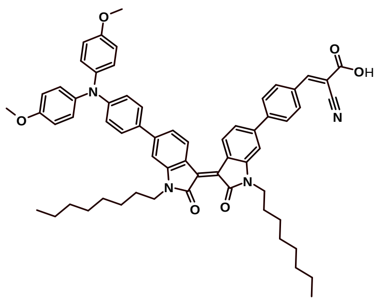
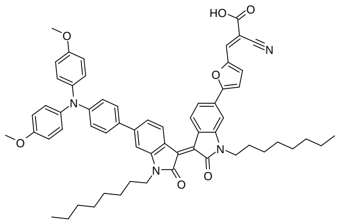
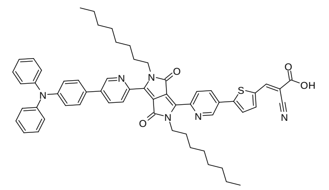
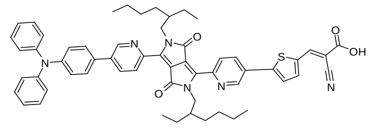
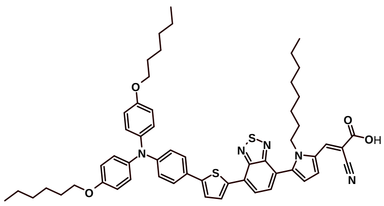
2. Conjunto de Estruturas e Grupos de Treino e Testes Empregados

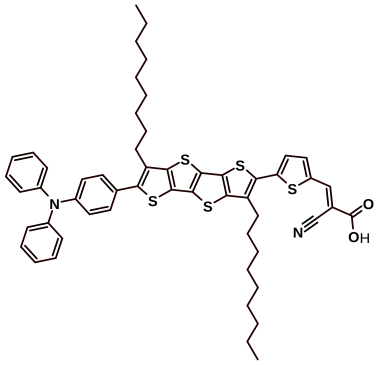
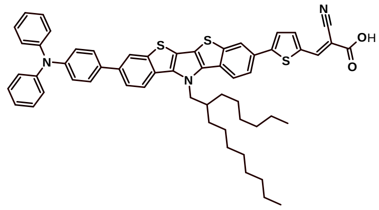
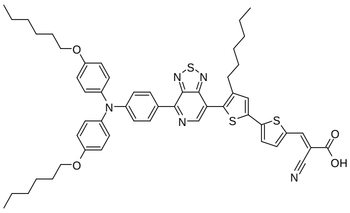
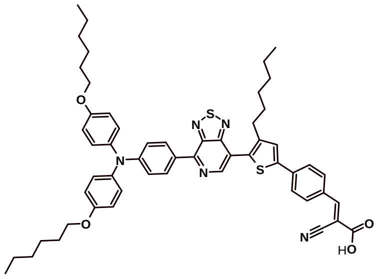
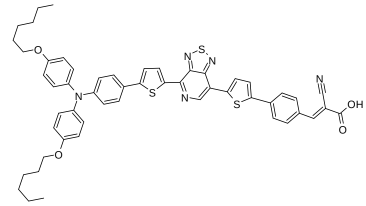
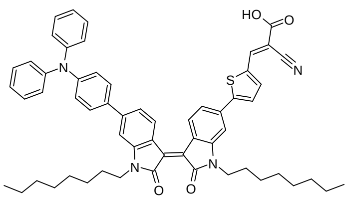
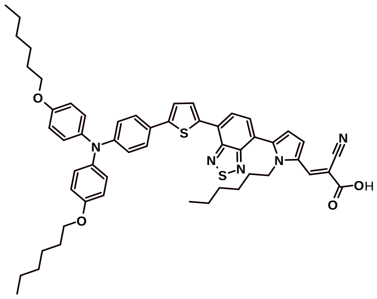
Tabela S2. Estruturas que compõem o conjunto de Treino e Teste

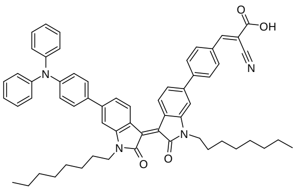
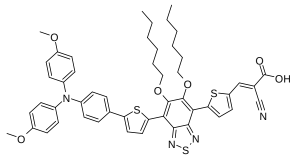
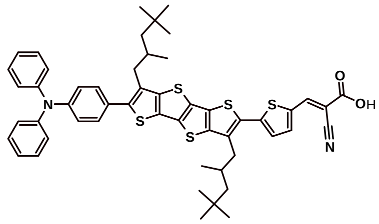
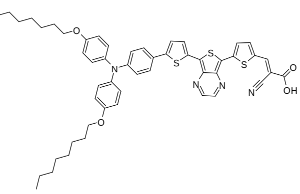
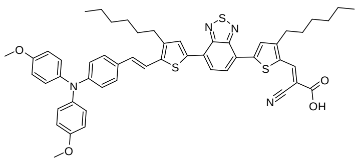
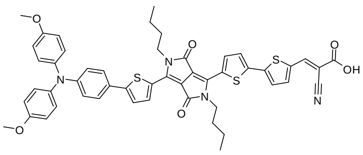
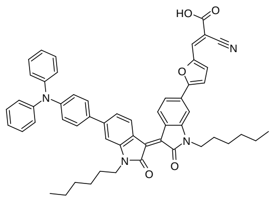
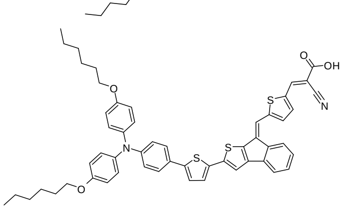
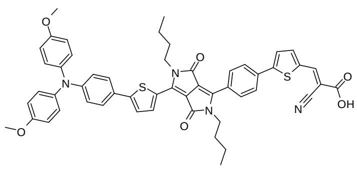
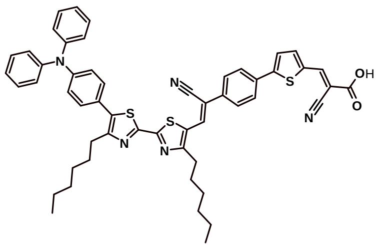
Grupo	Estruturas
Treino	dye46, dye5, dye200, dye26, dye136, dye98, dye40, dye124, dye15, dye88, dye79, dye49, dye6, dye19, dye126, dye17, dye56, dye7, dye128, dye60, dye4, dye67, dye83, dye8, dye52, dye166, dye102, dye28, dye90, dye94, dye74, dye133, dye35, dye54, dye18, dye190, dye70, dye3, dye131, dye2, dye100, dye109, dye30, dye104, dye29, dye84, dye82, dye81, dye73, dye43, dye45, dye139, dye105, dye183, dye137, dye16, dye176, dye20, dye63, dye65, dye14, dye103, dye89, dye95, dye33, dye34, dye127, dye198, dye97, dye192, dye37, dye177, dye93, dye118, dye99, dye27, dye39, dye11, dye130, dye72, dye75, dye61, dye51, dye44, dye167, dye141, dye57, dye68, dye10, dye85, dye147, dye117, dye86, dye9, dye171, dye78, dye48, dye155, dye87, dye62, dye143, dye173, dye101, dye92, dye25, dye50, dye148, dye47, dye41, dye64, dye116, dye182, dye186, dye21, dye1, dye69, dye142, dye123, dye150, dye199, dye58, dye76, dye174, dye180, dye135, dye42, dye110, dye59, dye184, dye149, dye13, dye23, dye71, dye169, dye111, dye144, dye197, dye114, dye96, dye159
Teste	dye12, dye22, dye24, dye31, dye32, dye36, dye38, dye53, dye55, dye66, dye77, dye80, dye91, dye106, dye107, dye108, dye112, dye113, dye115, dye119, dye120, dye121, dye122, dye125, dye129, dye132, dye134, dye138, dye140, dye145, dye146, dye151, dye152, dye153, dye154, dye156, dye157, dye158, dye160, dye161, dye162, dye163, dye164, dye165, dye168, dye170, dye172, dye175, dye178, dye179, dye181, dye185, dye187, dye188, dye189, dye191, dye193, dye194, dye195, dye196

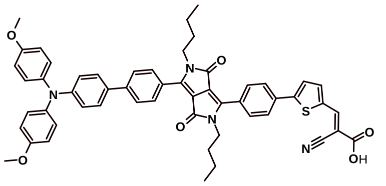
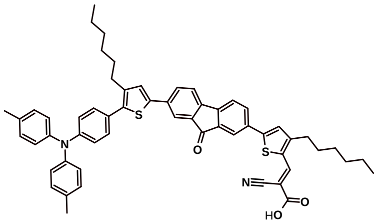
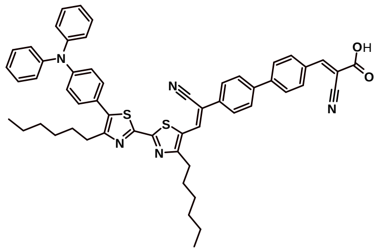
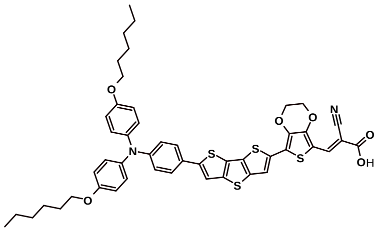
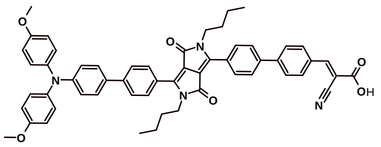
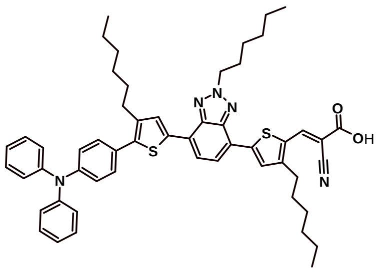
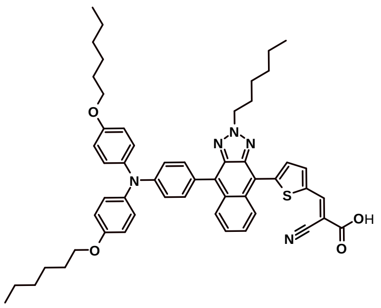
Table S3. Conjunto com as 200 estruturas empregadas na modelagem.

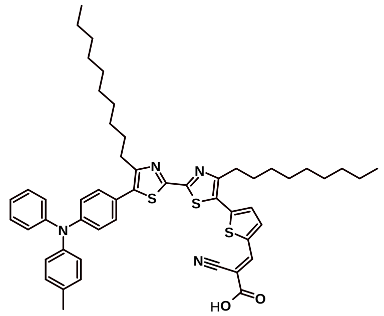
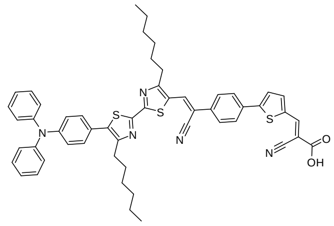
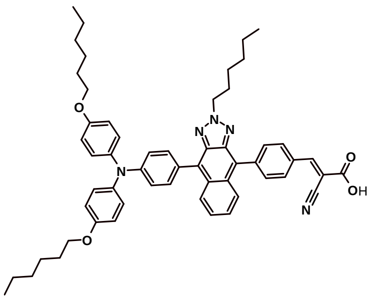
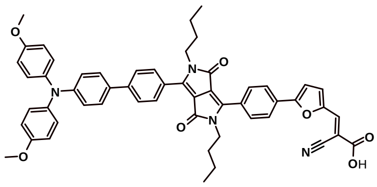
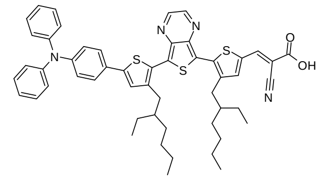
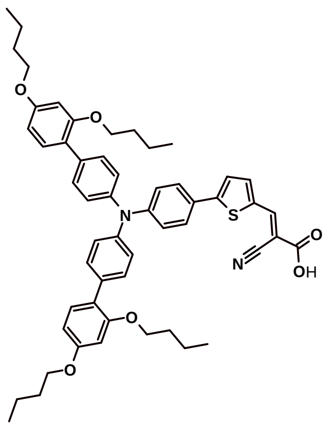
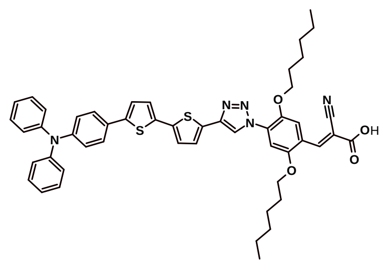
Name	Estrutura do Corante	ΔG_{inj}	%PCE	DOI
dye1		-1.75	7.57	10.1016/j.jpowsour.2014.08.030
dye2		-1.882	4.12	10.1016/j.jpowsour.2014.08.030
dye3		-1.516	5.1	10.1039/C5RA27288B
dye4		-1.446	4.59	10.1039/C5RA27288B
dye5		-1.792	7.25	10.1039/C8TA06258G
dye6		-1.993	5.04	10.1021/ol902973r
dye7		-1.127	4.81	10.1016/j.orgel.2012.05.013
dye8		-1.674	4.14	10.1016/j.dyepig.2016.04.020

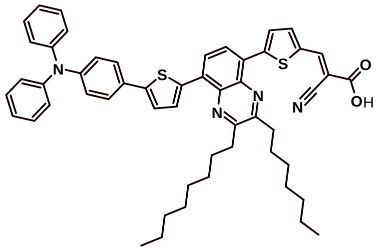
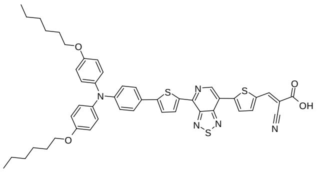
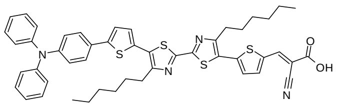
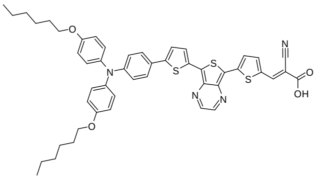
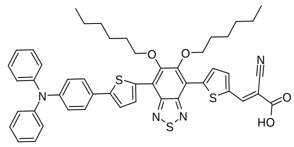
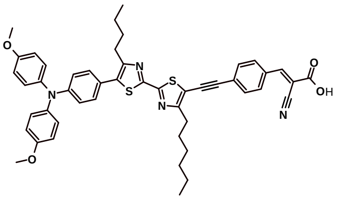
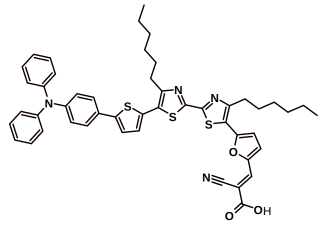
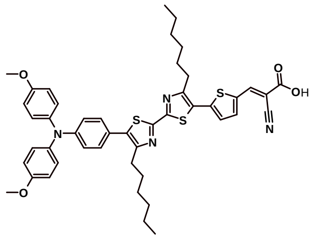
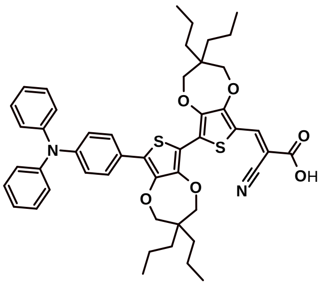
dye9		-1.756	1.96	10.1002/ajoc.201600100
dye10		-1.267	3.42	10.1016/j.orgel.2012.05.013
dye11		-1.624	4.36	10.1021/am300925e
dye12		-1.766	5.35	10.1021/am300925e
dye13		-1.631	4.41	10.1021/am300925e
dye14		-1.443	4.8	10.1039/C5RA27288B
dye15		-1.304	5.26	10.1039/C5RA27288B
dye16		-1.747	8.54	10.1039/C8TA06258G

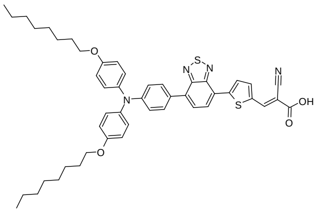
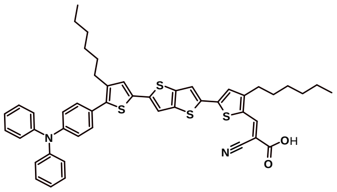
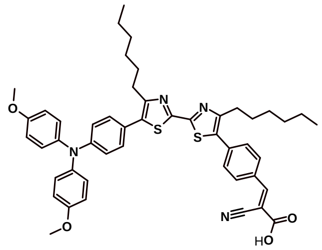
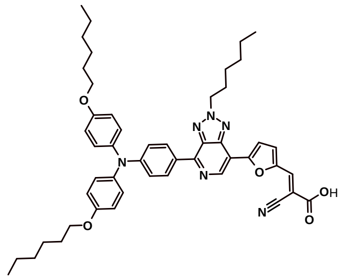
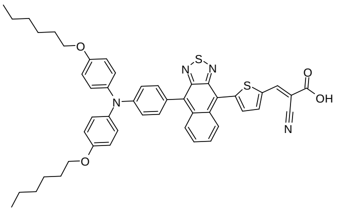
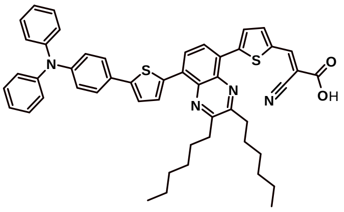
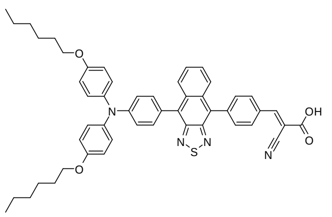
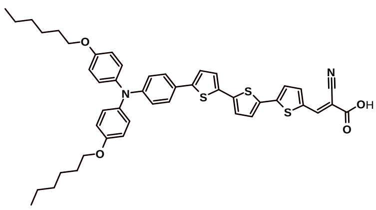
dye17		-1.752	7.6	10.1039/C7TA01825H
dye18		-1.999	5.72	10.1016/j.dyepig.2019.107676
dye19		-1.618	2.86	10.1039/C4TA05350H
dye20		-1.723	4.46	10.1039/C4TA05350H
dye21		-1.488	1.32	10.1039/C4TA05350H
dye22		-1.411	3.52	10.1021/am300925e
dye23		-1.742	6.94	10.1039/C8TA06258G

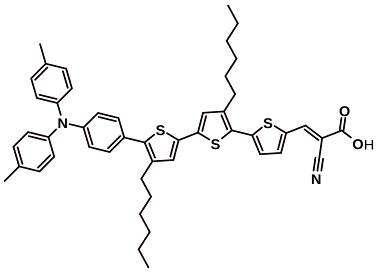
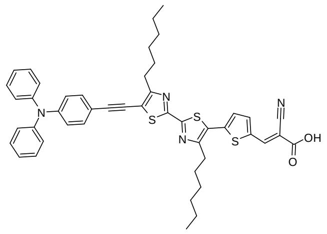
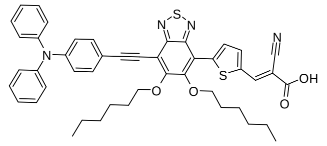
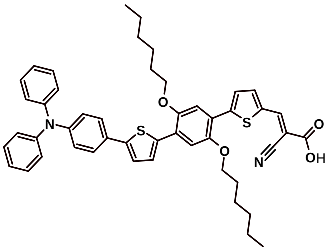
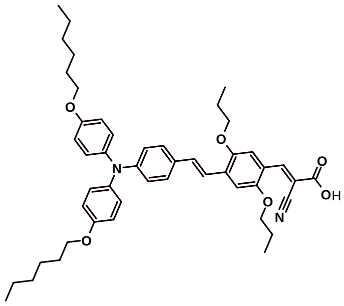
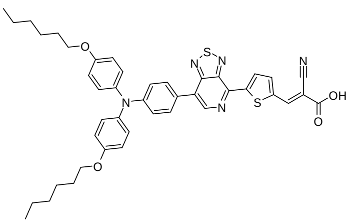
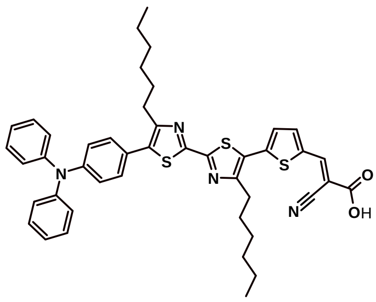
dye24		-1.536	3.33	10.1021/am300925e
dye25		-1.681	5.36	10.1039/c2jm30427a
dye26		-1.765	10.21	10.1039/C7TA01825H
dye27		-1.246	8.27	10.1021/cm301520z
dye28		-1.538	4.68	10.1002/asia.201000158
dye29		-1.381	1.45	10.1016/j.solener.2012.05.003
dye30		-1.395	3.92	10.1021/am300925e
dye31		-1.694	2.7	10.1002/ajoc.201600100
dye32		-1.393	0.43	10.1021/jp909786k
dye33		-1.8	3.69	10.1002/chem.201103702

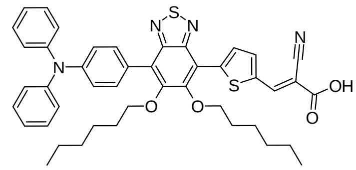
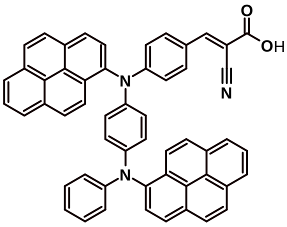
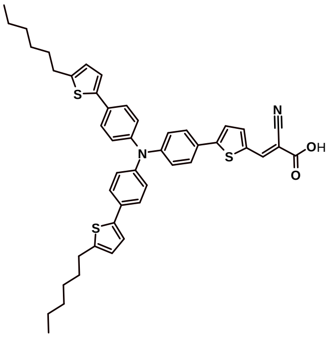
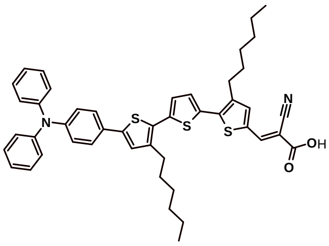
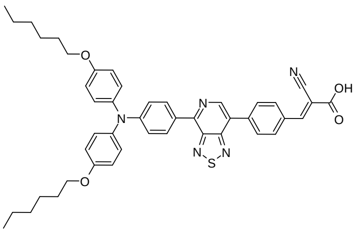
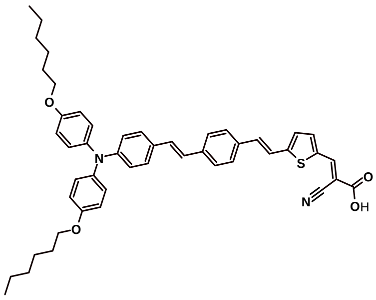
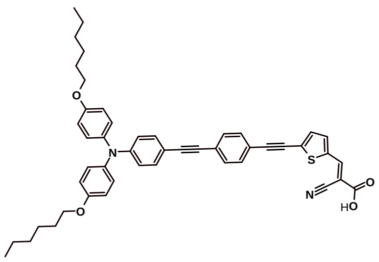
dye34		-1.822	3.44	10.1021/jp909786k
dye35		-2.057	5.33	10.1016/j.jpowsour.2013.08.034
dye36		-1.784	5.49	10.1002/chem.201103702
dye37		-2.006	4.18	10.1016/j.tet.2012.04.113
dye38		-1.945	6.03	10.1016/j.dyepig.2011.09.009
dye39		-1.756	5.89	10.1002/asia.201201173
dye40		-1.878	7.23	10.1021/acsami.6b00806

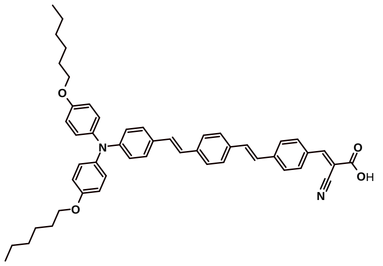
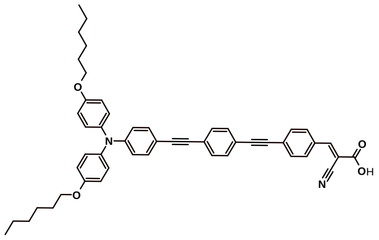
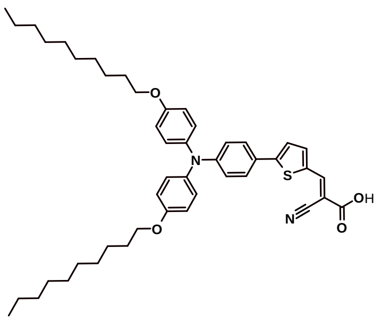
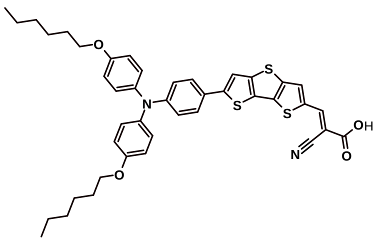
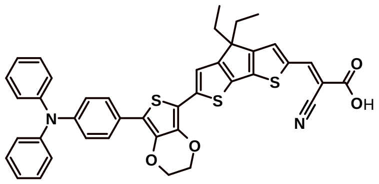
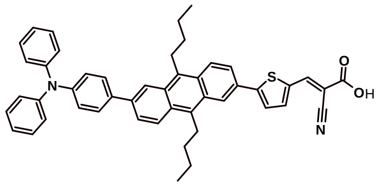
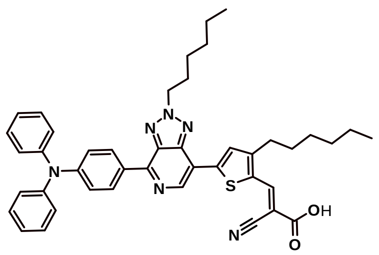
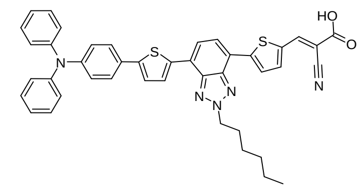
dye41		-1.725	2.98	10.1016/j.dyepig.2012.10.002
dye42		-1.659	3.58	10.1002/chem.201103702
dye43		-2.139	7.09	10.1021/acsami.6b00806
dye44		-1.851	4.43	10.1016/j.dyepig.2011.09.009
dye45		-1.27	2.52	10.1021/cm301520z
dye46		-2.133	6	10.1039/B911397P
dye47		-2.348	4.81	10.1016/j.dyepig.2015.02.005

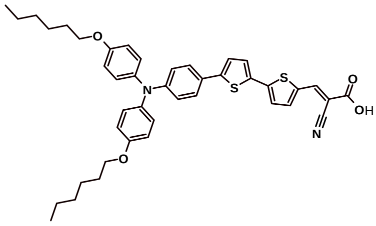
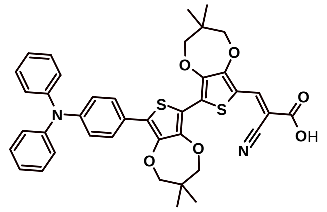
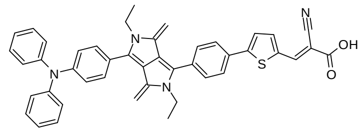
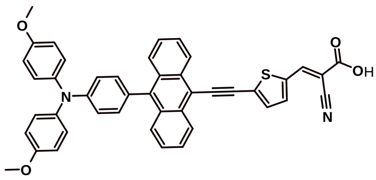
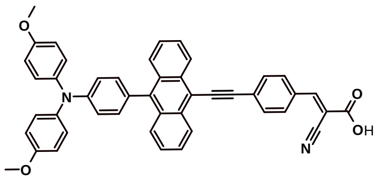
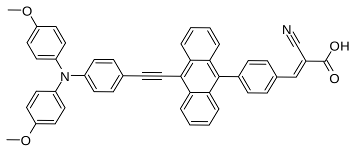
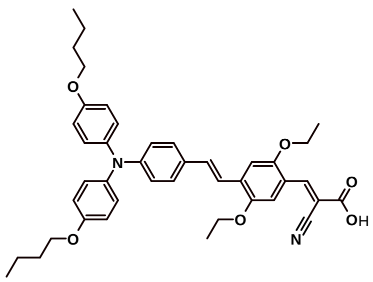
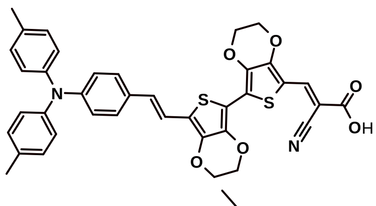
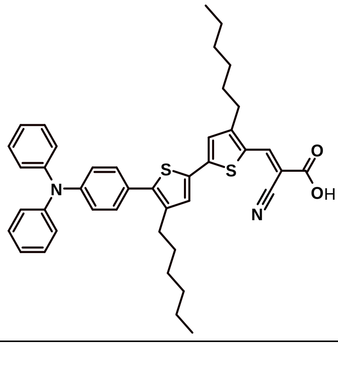
dye48		-1.868	7.78	10.1016/j.dyepig.2017.05.054
dye49		-1.351	0.69	10.1016/j.orgel.2013.11.031
dye50		-1.677	7.51	10.1002/chem.201103702
dye51		-1.252	7.4	10.1021/cm301520z
dye52		-1.51	6.72	10.1039/c2jm30427a
dye53		-2.1	5.05	10.1039/c0jm03811c
dye54		-1.702	7.11	10.1002/chem.201103702
dye55		-1.418	4.448	10.1039/c0jm03811c
dye56		-1.917	5.3	10.1021/ol902973r

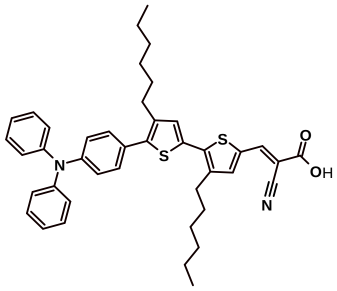
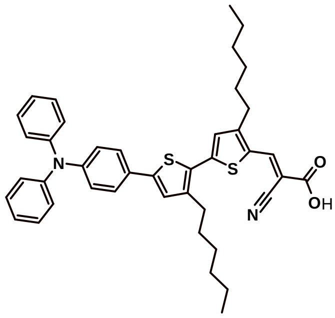
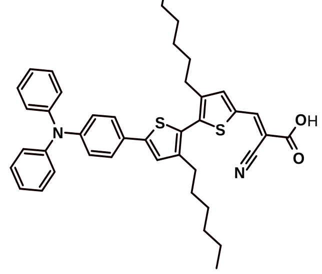
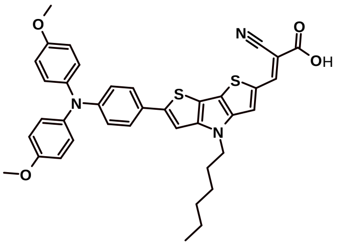
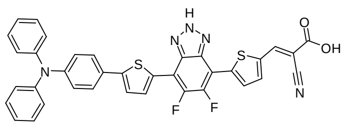
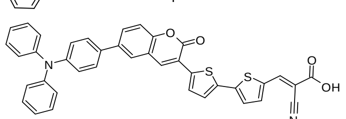
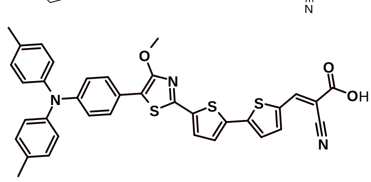
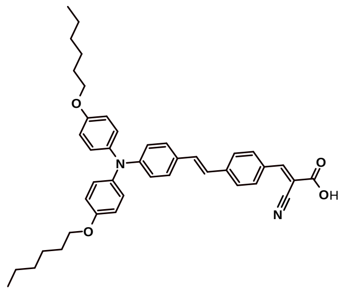
dye57		-1.54	5.67	10.1016/j.electacta.2015.05.003
dye58		-1.659	5.1	10.1016/j.orgel.2017.10.003
dye59		-1.93	4.2	10.1039/c0jm03811c
dye60		-1.879	7.22	10.1021/acsami.5b07205
dye61		-1.76	1.94	10.1021/acsami.6b00806
dye62		-1.917	7.42	10.1016/j.dyepig.2016.04.001
dye63		-2.211	6.37	10.1021/acsami.6b00806
dye64		-1.607	3.4	10.1021/cm302250y

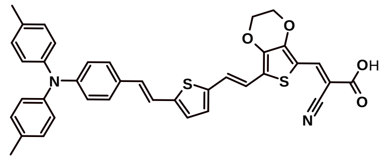
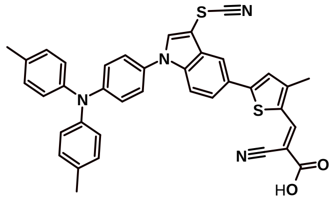
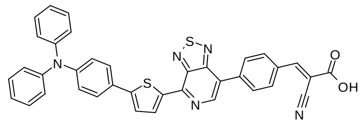
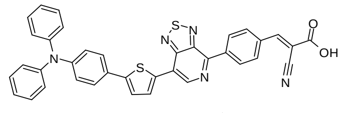
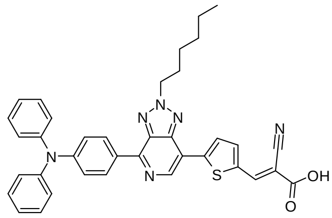
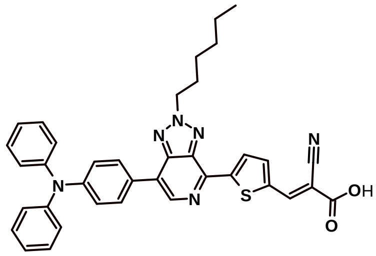
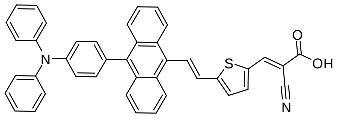
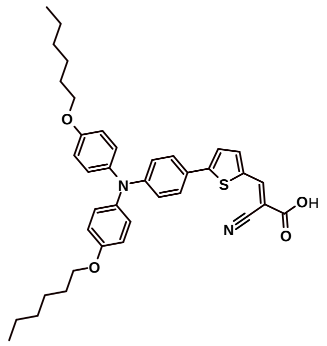
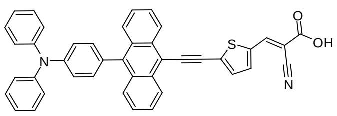
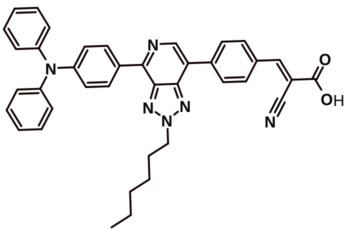
dye65		-1.998	5.3	10.1016/j.jpowsour.2020.227776
dye66		-1.682	5.6	10.1039/c0jm03811c
dye67		-2.216	6.22	10.1039/c2jm30427a
dye68		-2.085	6.53	10.1016/j.dyepig.2016.04.001
dye69		-2.057	7.02	10.1016/j.jphotochem.2011.09.019
dye70		-1.662	4.2	10.1016/j.dyepig.2013.11.001
dye71		-1.569	5.73	10.1039/c0jm03811c

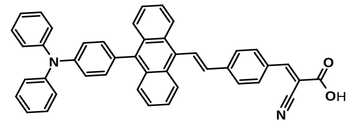
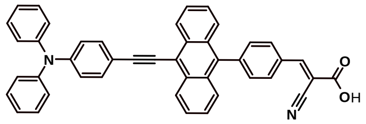
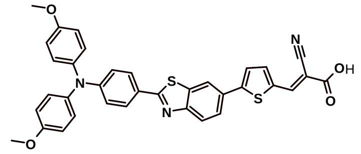
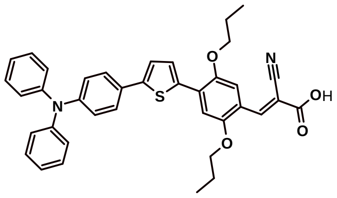
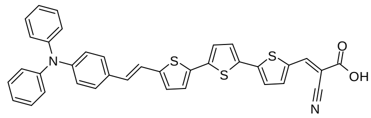
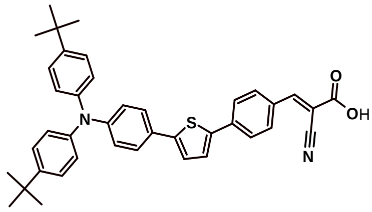
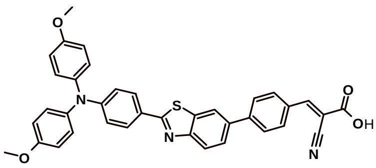
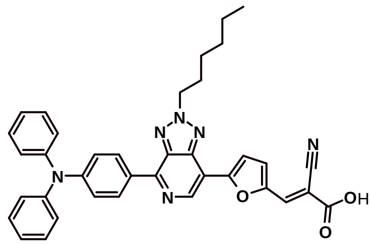
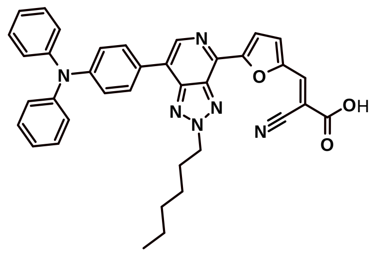
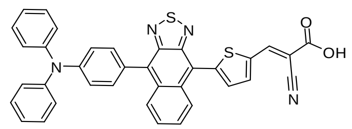
dye72		-1.777	5.57	10.1039/c2jm30427a
dye73		-1.942	2.88	10.1002/asia.201100849
dye74		-2.093	5.63	10.1016/j.synthmet.2013.02.010
dye75		-1.988	4.25	10.1016/j.dyepig.2009.04.005
dye76		-1.904	1.26	10.1016/j.orgel.2013.11.031
dye77		-1.81	4.16	10.1039/C7NJ00413C
dye78		-2.098	3.43	10.1039/C7NJ00413C

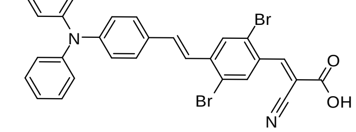
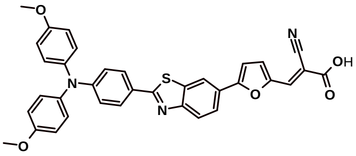
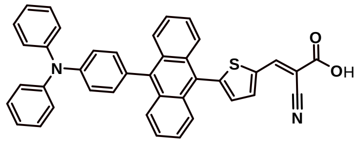
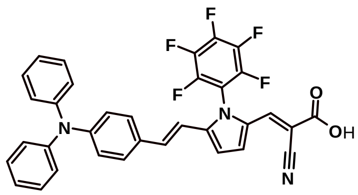
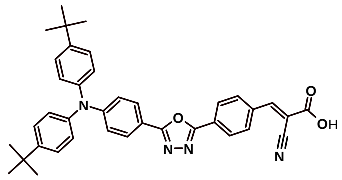
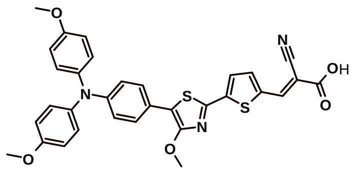
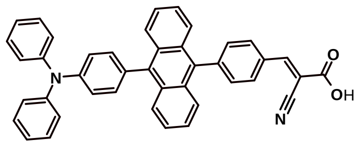
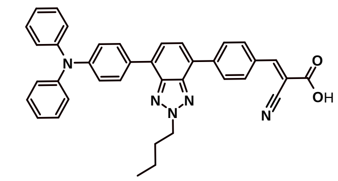
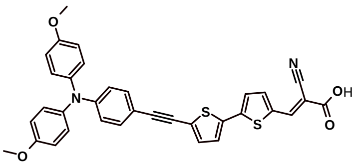
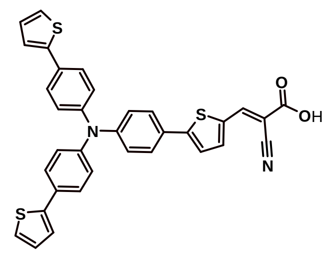
dye79		-2.163	4.63	10.1039/C7NJ00413C
dye80		-1.888	4.17	10.1039/C7NJ00413C
dye81		-1.805	6.04	10.1021/jp2054519
dye82		-1.901	3.57	10.1016/j.jphotochem.2013.10.016
dye83		-1.769	5.4	10.1016/j.dyepig.2011.09.019
dye84		-1.609	5.6	10.1016/j.tet.2013.11.072
dye85		-1.669	7.92	10.1021/acsami.5b07205
dye86		-1.462	6.2	10.1002/asia.201201173

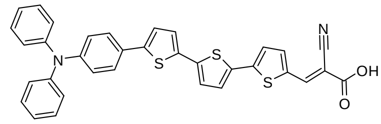
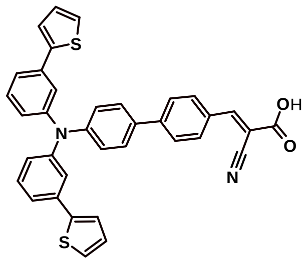
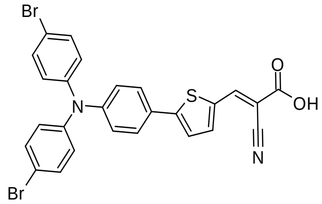
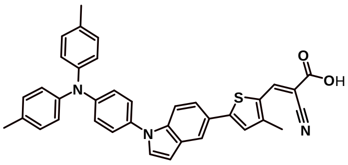
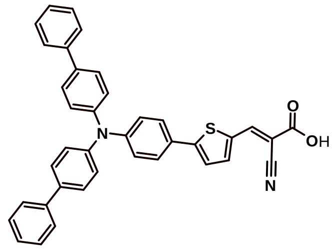
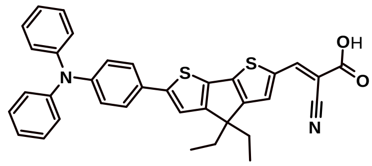
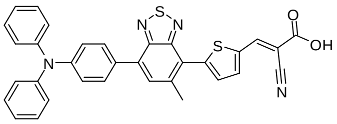
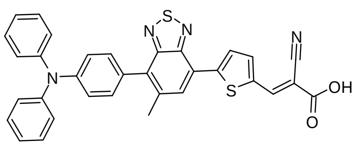
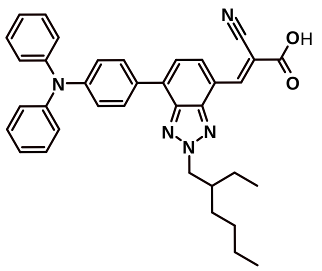
dye87		-2.152	5.33	10.1021/acsami.6b10162
dye88		-1.968	4.45	10.1021/ol902973r
dye89		-1.602	3.51	10.1039/C8NJ00847G
dye90		-1.731	6.82	10.1021/jp101238k
dye91		-1.916	7.03	10.1021/jp101238k
dye92		-1.684	5.66	10.1021/jp101238k
dye93		-2.206	4.02	10.1002/cjoc.201200091
dye94		-1.948	3.59	10.1039/B815649B
dye95		-1.867	4.96	10.1016/j.jpowsour.2013.01.127

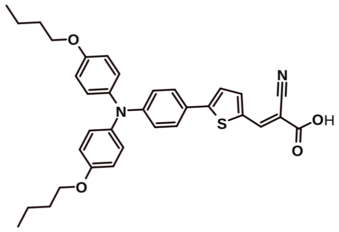
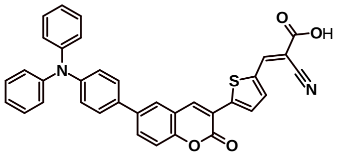
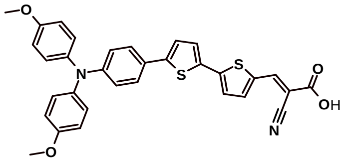
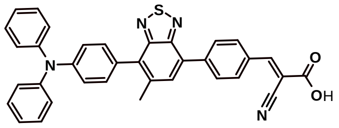
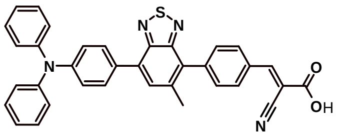
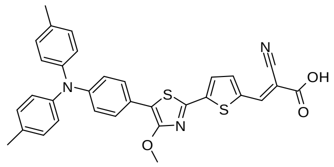
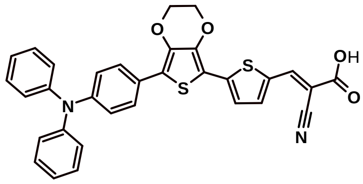
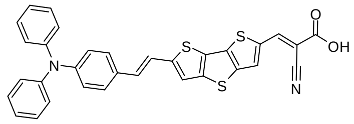
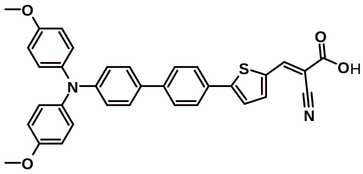
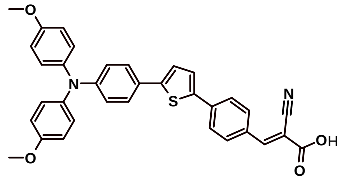
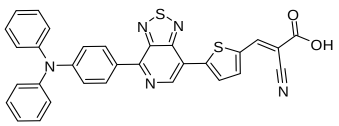
dye96		-1.947	5.78	10.1016/j.jpowsour.2013.01.127
dye97		-1.923	5.86	10.1016/j.jpowsour.2013.01.127
dye98		-2.124	4	10.1016/j.jpowsour.2013.01.127
dye99		-2.023	5.1	10.1021/acs.jpcc.6b06604
dye100		-1.631	6.01	10.1002/asia.201201173
dye101		-1.676	4.4	10.1039/C6PP00410E
dye102		-1.713	0.36	10.1016/j.dyepig.2012.02.014
dye103		-2.171	6.91	10.1016/j.jphotochem.2011.09.019

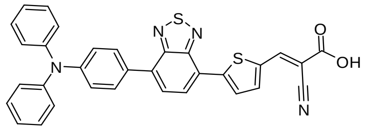
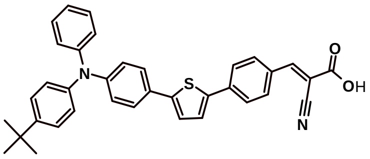
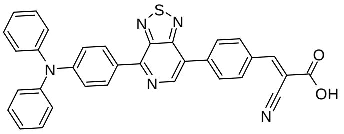
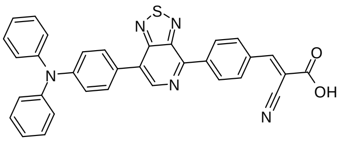
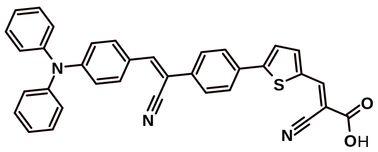
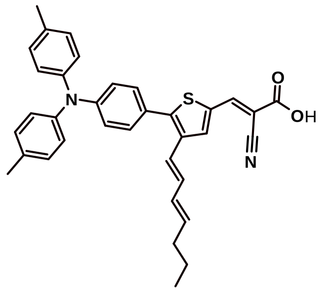
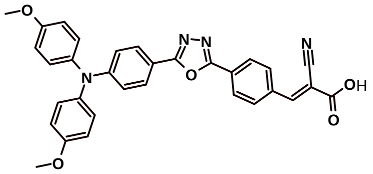
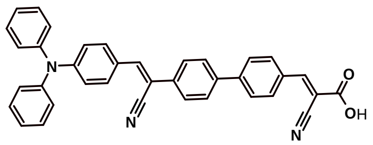
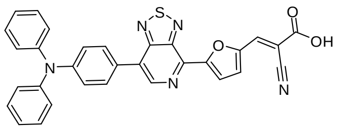
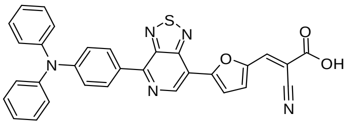
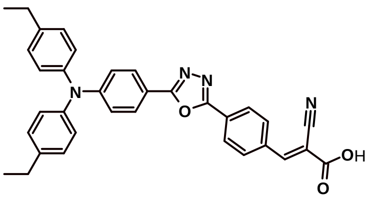
dye104		-1.794	6.03	10.1039/B815649B
dye105		-2.037	6.74	10.1016/j.jpowsour.2013.09.106
dye106		-1.415	3.06	10.1016/j.orgel.2013.11.031
dye107		-1.335	1.06	10.1016/j.orgel.2013.11.031
dye108		-1.643	6.64	10.1021/acsami.5b07205
dye109		-1.715	6.12	10.1021/acsami.5b07205
dye110		-1.652	4.86	10.1021/jp101238k
dye111		-2.02	5.64	10.1021/jp2054519
dye112		-1.484	4.5	10.1021/jp101238k
dye113		-1.958	4.92	10.1021/acsami.5b07205

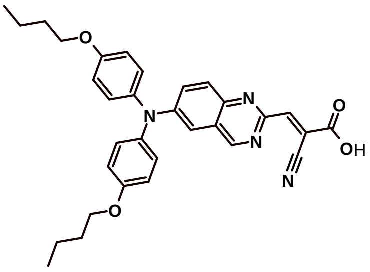
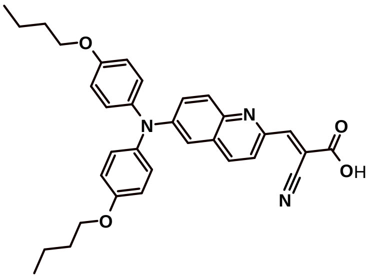
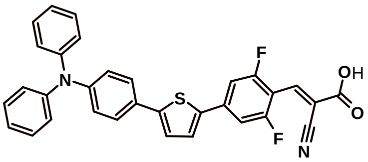
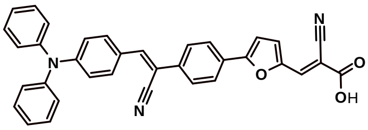
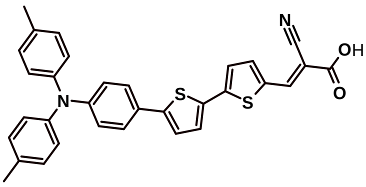
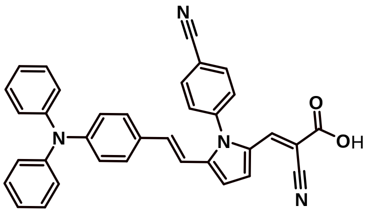
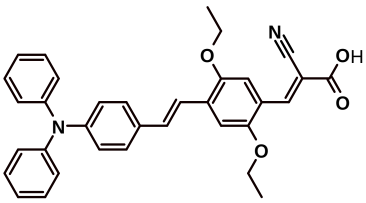
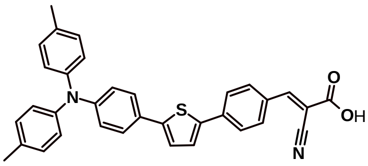
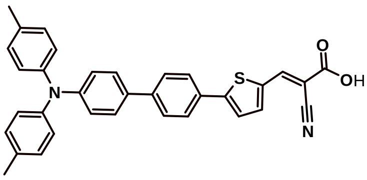
dye114		-1.849	5.14	10.1021/jp101238k
dye115		-1.978	3.93	10.1021/jp101238k
dye116		-2.078	4.16	10.1007/s11426-012-4758-8
dye117		-2.002	6.4	10.1007/s10853-011-5971-0
dye118		-1.657	2.75	10.1021/jp800953s
dye119		-2.095	6.14	10.1002/asia.201100777
dye120		-2.394	3.15	10.1007/s11426-012-4758-8
dye121		-1.781	7.22	10.1021/acsami.5b07205
dye122		-1.795	5.45	10.1021/acsami.5b07205
dye123		-1.231	1.17	10.1021/acsami.6b00806

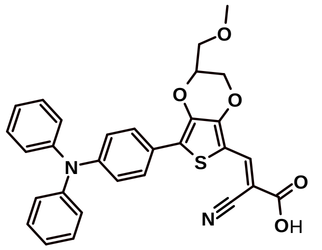
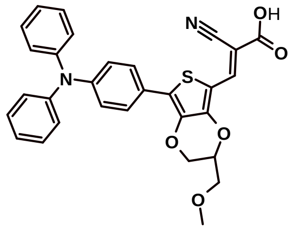
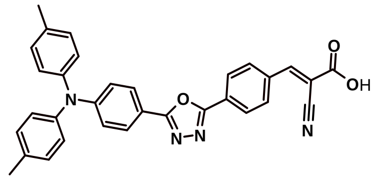
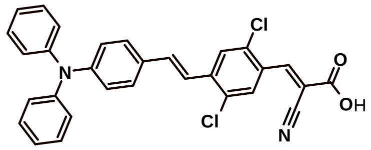
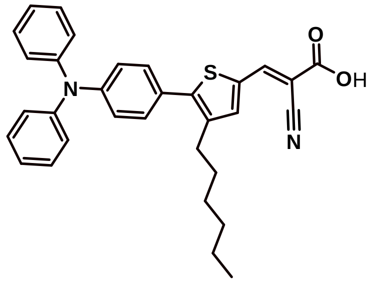
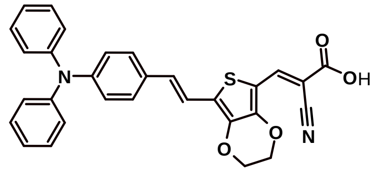
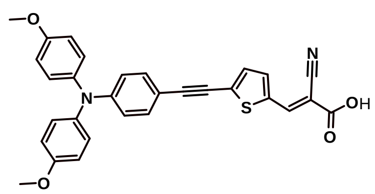
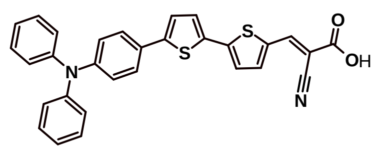
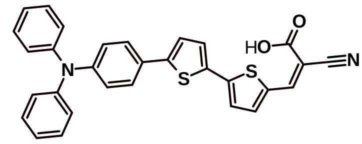
dye124		-1.69	4.36	10.1021/jp800953s
dye125		-2.129	4.12	10.1007/s11426-012-4758-8
dye126		-2.253	2.91	10.1021/jp101238k
dye127		-1.862	6.23	10.1016/j.dyepig.2013.05.030
dye128		-2.119	3.21	10.1016/j.synthmet.2011.06.001
dye129		-1.733	0.41	10.1016/j.dyepig.2012.02.014
dye130		-2.209	3.09	10.1021/jp101238k
dye131		-2.154	6.19	10.1016/j.dyepig.2018.05.044
dye132		-1.832	4.98	10.1039/C0NJ00653J
dye133		-1.909	3.45	10.1016/j.synthmet.2013.02.010

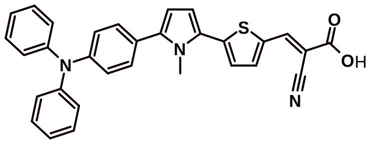
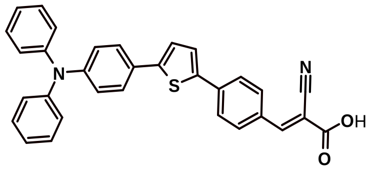
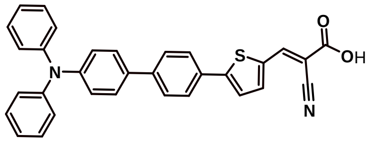
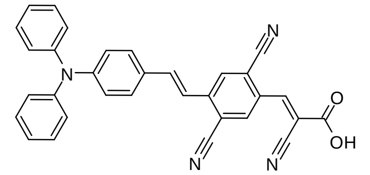
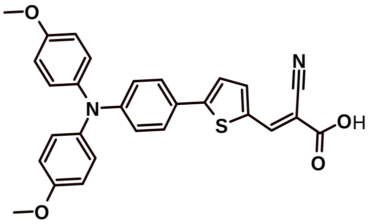
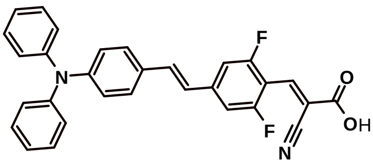
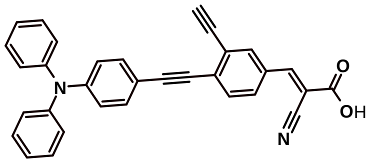
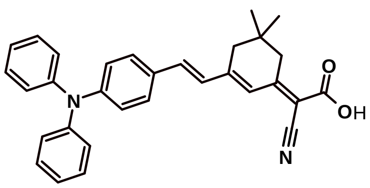
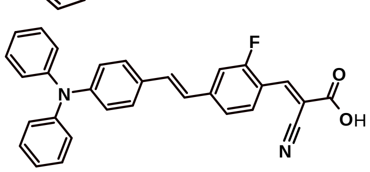
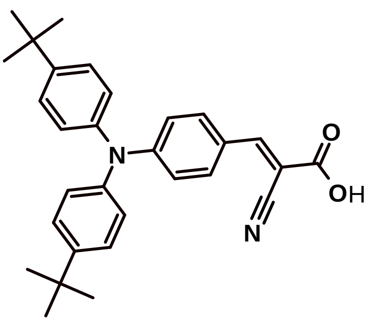
dye134		-1.67	3.21	10.1016/j.dyepig.2009.04.005
dye135		-2.238	5.24	10.1039/C2CP42993D
dye136		-1.666	2.54	10.1016/j.cap.2010.11.052
dye137		-2.181	5.53	10.1016/j.jpowsour.2013.09.106
dye138		-1.848	5.25	10.1016/j.synthmet.2013.02.010
dye139		-1.714	5.8	10.1016/j.dyepig.2011.09.019
dye140		-1.642	2.71	10.1016/j.electacta.2019.02.077
dye141		-1.604	4.33	10.1016/j.electacta.2019.02.077
dye142		-1.814	5.67	10.1039/c5cc07105d

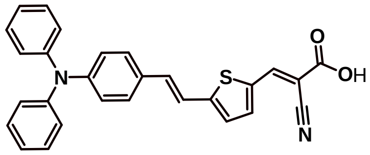
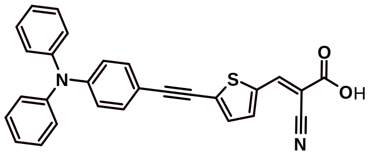
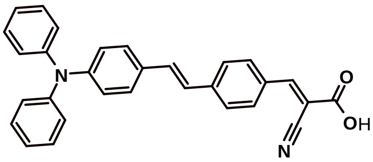
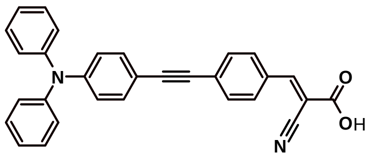
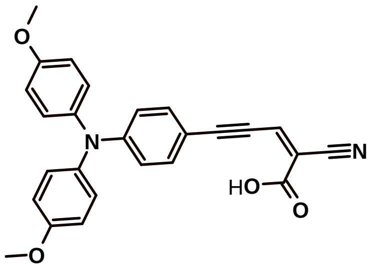
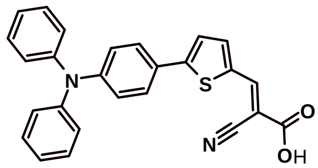
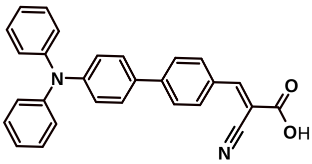
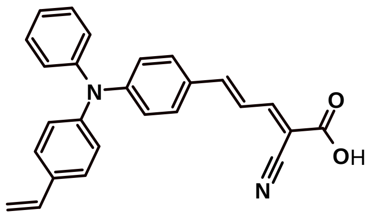
dye143		-2.031	6.65	10.1016/j.dyepig.2010.03.034
dye144		-1.9	4.52	10.1039/C6PP00410E
dye145		-1.908	5.61	10.1016/j.tsf.2014.03.010
dye146		-1.973	3.94	10.1016/j.electacta.2019.02.077
dye147		-1.997	0.68	10.1016/j.electacta.2019.02.077
dye148		-1.655	0.44	10.1016/j.dyepig.2012.02.014
dye149		-1.82	4.88	10.1016/j.dyepig.2013.04.031
dye150		-1.699	2.76	10.1021/jp800953s
dye151		-2.267	4.09	10.1016/j.tet.2009.09.036
dye152		-2.197	5.98	10.1016/j.tet.2009.09.036
dye153		-1.171	1.16	10.1016/j.orgel.2013.11.031

dye154		-1.433	5.01	10.1039/c2jm30427a
dye155		-2.065	5.43	10.1002/asia.201100777
dye156		-1.424	2.88	10.1016/j.orgel.2013.11.031
dye157		-1.436	3.87	10.1016/j.orgel.2013.11.031
dye158		-1.724	3.45	10.1016/j.jphotochem.2014.11.018
dye159		-1.97	6.93	10.1016/j.dyepig.2015.09.025
dye160		-2.213	2.85	10.1016/j.synthmet.2011.06.001
dye161		-1.963	3.52	10.1016/j.jphotochem.2014.11.018
dye162		-1.312	0.19	10.1016/j.orgel.2013.11.031
dye163		-1.199	0.82	10.1016/j.orgel.2013.11.031
dye164		-2.107	3.08	10.1016/j.synthmet.2011.06.001

dye165		-1.963	1.81	10.1016/j.dyepig.2015.09.002
dye166		-2.067	2.51	10.1016/j.dyepig.2015.09.002
dye167		-1.994	4.8	10.1007/s10853-011-5971-0
dye168		-1.742	1.32	10.1016/j.jphotochem.2014.11.018
dye169		-1.793	6.13	10.1016/j.tsf.2014.03.010
dye170		-1.876	5.71	10.1016/j.dyepig.2013.05.030
dye171		-1.988	4.23	10.1002/cjoc.201200091
dye172		-2.096	6.05	10.1016/j.tet.2009.09.036
dye173		-2.156	5.26	10.1016/j.tet.2009.09.036

dye174		-1.976	5.3	10.1039/C4TA03451A
dye175		-1.965	4.9	10.1039/C4TA03451A
dye176		-2.114	3.11	10.1016/j.synthmet.2011.06.001
dye177		-1.722	3.86	10.1021/jp800953s
dye178		-1.977	4.02	10.1016/j.dyepig.2009.04.005
dye179		-1.858	4.44	10.1002/aenm.201200435
dye180		-1.892	3.86	10.1039/C0NJ00653J
dye181		-1.72	4.36	10.1021/ol902973r
dye182		-1.72	6.15	10.1021/cm702631r

dye183		-1.884	4.79	10.1021/jp801036s
dye184		-2.019	5.25	10.1016/j.tet.2009.09.036
dye185		-2.064	5.14	10.1016/j.tet.2009.09.036
dye186		-1.334	0.44	10.1021/jp800953s
dye187		-1.976	4.99	10.1021/jp2054519
dye188		-1.912	3.62	10.1016/j.jphotochem.2011.12.013
dye189		-1.921	3.26	10.1039/c5ra25938j
dye190		-1.875	5.77	10.1021/jo800159t
dye191		-1.867	5.19	10.1016/j.jphotochem.2011.12.013
dye192		-2.074	3.37	10.1246/cl.2010.864

dye193		-1.726	4.8	10.1016/j.dyepig.2009.06.014
dye194		-1.722	5	10.1021/jp102697p
dye195		-1.972	5.33	10.1021/jp800953s
dye196		-1.996	4.3	10.1021/jp102697p
dye197		-2.177	3.21	10.1039/C0NJ00653J
dye198		-1.808	4.7	10.1016/j.synthmet.2013.02.010
dye199		-2.179	4.06	10.1021/jp102697p
dye200		-1.844	4.82	10.1021/jp076992d