Molecular design of organic photovoltaic donors and non-fullerene acceptors: machine learning combined genetic algorithm approach

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Table S1 Introduced 43 molecular structure descriptors for the two algorithms and adopted the 10-fold cross-validation method to optimize the PCE prediction in order to obtain the best hyperparameters.

Models	Best hyperparameters（PCE）
RF	bootstrap= True max_depth=43 max_features='log2' min_samples_leaf'=1 min_samples_split=3 n_estimators=231
ETR	bootstrap=False max_depth=33 max_features='sqrt' min_samples_leaf=1 min_samples_split=5 n_estimators=231

Table S2 Introduced 43 molecular structure descriptors for the two algorithms and adopted the 10-fold cross-validation method to optimize the V_{OC} prediction in order to obtain the best hyperparameters.

Models	Best hyperparameters（V_{OC}）
RF	bootstrap= False max_depth=29 max_features='log2' min_samples_leaf'=1 min_samples_split=3 n_estimators=231
ETR	bootstrap=False

	max_depth=14 max_features='sqrt' min_samples_leaf=1 min_samples_split=5 n_estimators=10

Table S3 Introduced 43 molecular structure descriptors for the two algorithms and adopted the 10-fold cross-validation method to optimize the J_{SC} prediction in order to obtain the best hyperparameters.

Models	Best hyperparameters（J_{SC}）
RF	bootstrap= True max_depth=40 max_features='log2' min_samples_leaf'=1 min_samples_split=3 n_estimators=231
ETR	bootstrap=False max_depth=14 max_features='log2' min_samples_leaf=1 min_samples_split=3 n_estimators=452

Table S4 Introduced 43 molecular structure descriptors for the two algorithms and adopted the 10-fold cross-validation method to optimize the FF prediction in order to obtain the best hyperparameters.

Models	Best hyperparameters（FF）
RF	bootstrap= False

		max_depth=18 max_features='log2' min_samples_leaf'=1 min_samples_split=7 n_estimators=231
	ETR	bootstrap=False max_depth=40 max_features='sqrt' min_samples_leaf=1 min_samples_split=7 n_estimators=10

Table S5 The RF predicted values, experimental values, and errors of V_{OC} for 5 donor-acceptor pairs in the database.

Donor	Acceptor	Experimental V_{OC} (V)	Predictive V_{OC} (V)	Absolute error	Relative error
D18	BTP-eC11	0.86	0.86	0	0
PM6	BTP-C6Ph	0.84	0.85	0.01	0.01
B1	BO-2Cl	0.86	0.85	0.01	0.01
BO2Cl	IT-4F	0.83	0.83	0	0
PBDB-PSF	ITIC	0.99	0.96	0.03	0.03

Table S6 The RF predicted values, experimental values, and errors of J_{SC} for 5 donor-acceptor pairs in the database.

Donor	Acceptor	Experimental J_{SC} (mA/cm^2)	Predictive J_{SC} (mA/cm^2)	Absolute error	Relative error
D18	BTP-eC11	27.10	26.75	0.35	0.01
PM6	BTP-C6Ph	24.30	24.32	0.02	0

B1	BO-2Cl	21.87	22.51	0.64	0.03
BO2Cl	IT-4F	19.90	19.63	0.27	0.01
PBDB-PSF	ITIC	16.99	15.53	1.46	0.09

Table S7 The RF predicted values, experimental values, and errors of FF for 5 donor-acceptor pairs in the database.

Donor	Acceptor	Experimental FF (%)	Predictive FF (%)	Absolute error	Relative error
D18	BTP-eC11	72.70	72.78	0.08	0
PM6	BTP-C6Ph	76.20	75.34	0.86	0.01
B1	BO-2Cl	73.00	71.32	1.68	0.02
BO2Cl	IT-4F	65.40	64.84	0.56	0.01
PBDB-PSF	ITIC	58.73	63.18	4.45	0.08

Table S8 The RF predicted values, experimental values, and errors of V_{OC} for 5 donor-acceptor pairs outside the database.

Donor	Acceptor	Experimental V_{OC} (V)	Predictive V_{OC} (V)	Absolute error	Relative error
PM6	BTA-UD-4F	0.81	0.84	0.03	0.04
PBDP-2Cl	BTIC-BO-4Cl	0.88	0.83	0.05	0.06
PTQ10	BTP-4F-12	0.86	0.84	0.02	0.02
PBDB-T	ITIC-m	0.94	0.95	0.01	0.01
PTPTz-Th-IDT-	Y6	0.81	0.78	0.03	0.04

Table S9 The RF predicted values, experimental values, and errors of J_{SC} for 5 donor-acceptor pairs outside the database.

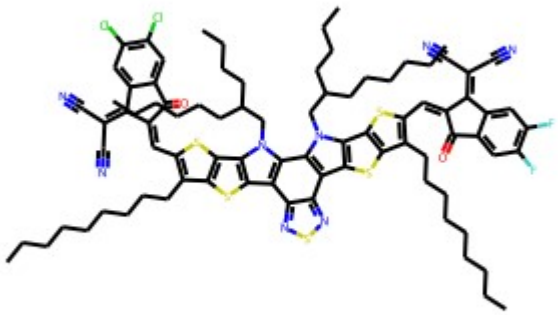
Donor	Acceptor	Experimental J_{SC} (mA/cm^2)	Predictive J_{SC} (mA/cm^2)	Absolute error	Relative error
PM6	BTA-UD-4F	24.98	24.23	0.75	0.03
PBDP-2Cl	BTIC-BO-4Cl	24.41	25.71	1.30	0.05
PTQ10	BTP-4F-12	22.15	21.92	0.23	0.01
PBDB-T	ITIC-m	16.25	15.70	0.55	0.03
PTPTz-Th-IDT-C12	Y6	19.50	21.58	2.08	0.11

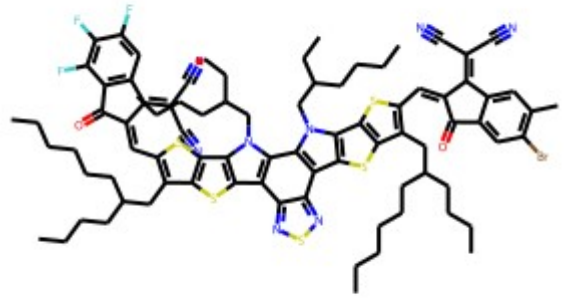
Table S10 The RF predicted values, experimental values, and errors of FF for 5 donor-acceptor pairs outside the database.

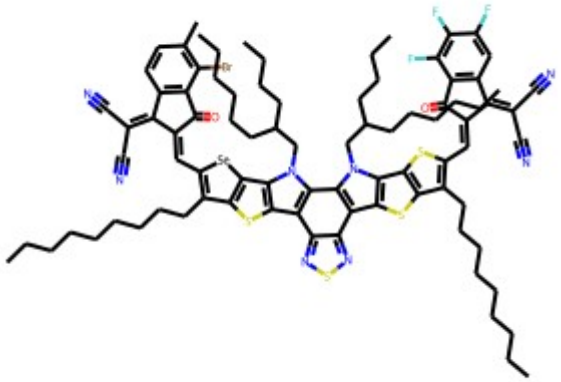
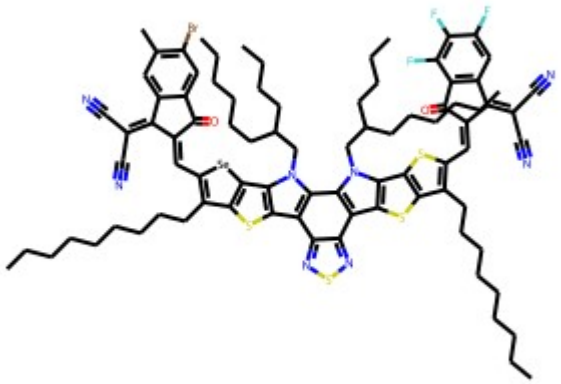
Donor	Acceptor	Experimental FF (%)	Predictive FF (%)	Absolute error	Relative error
PM6	BTA-UD-4F	67.98	73.67	5.69	0.08
PBDP-2Cl	BTIC-BO-4Cl	62.49	69.50	7.01	0.11
PTQ10	BTP-4F-12	62.55	64.03	1.48	0.02
PBDB-T	ITIC-m	67	62.55	4.45	0.07

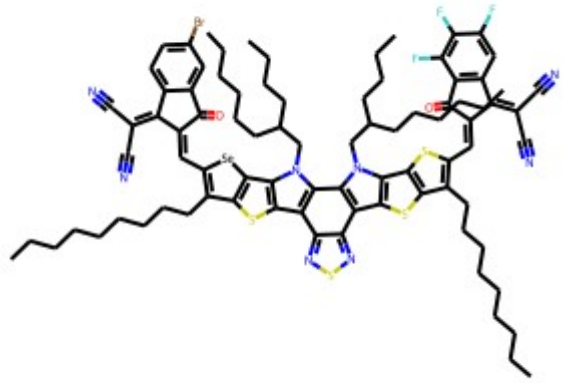
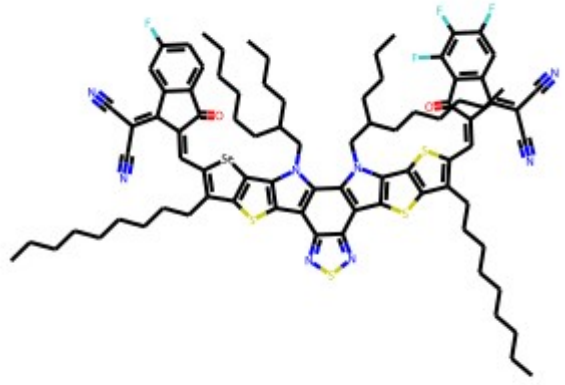
PTPTz-Th-IDT-C12	Y6	55	56.44	1.44	0.03

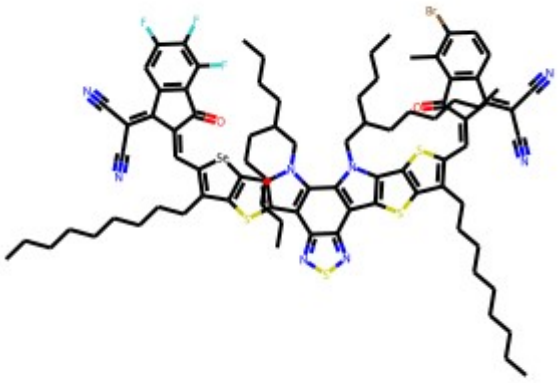
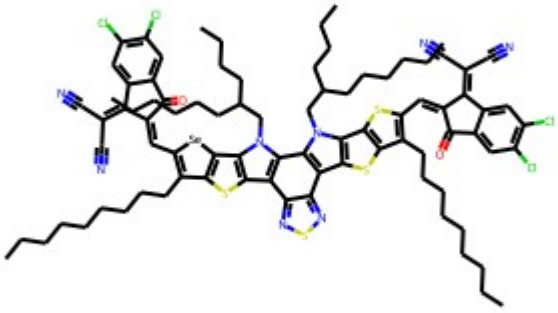
Table S11: The 32 A_1-D-A_2 type acceptor molecules with the higher PCE in the 100th generation.

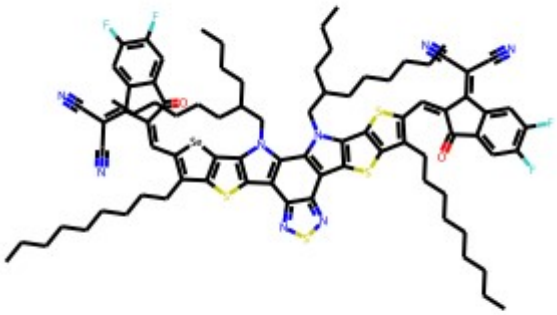
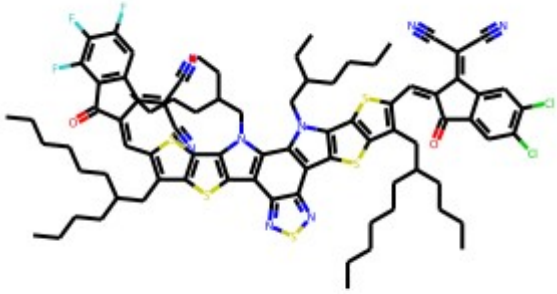
serial number	Designed acceptor molecule	Donor molecule	PCE Prediction
1	 CCCCCCCCc1c(C=C2C(=O)c3cc(F)c(F)cc3C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCC)c(C=C7C(=O)c8cc(Cl)c(Cl)cc8C7=C(C#N)C#N)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	16.94

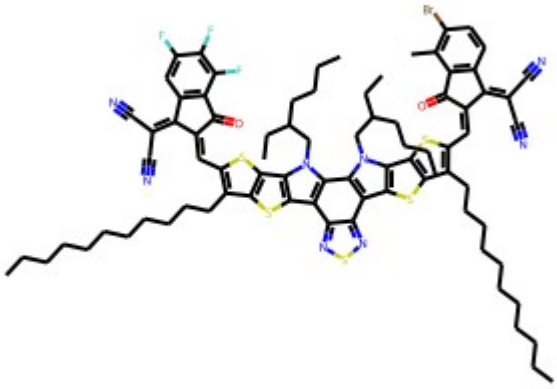
2	 C CCCCCC(CCCC)Cc1c(C=C2C(=O)c3c(cc(F)c(F)c3F)C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CC(CCCC)CCCCCC)c(C=C7C(=O)c8c(ccc(C)c8Br)C7=C(C#N)C#N)sc6c5n(CC(CC)CCCC)c4c3n(CC(CC)CCCC)c21	D18	16.90
3	 C CCCCCC(CCCC)Cc1c(C=C2C(=O)c3cc(Br)c(C)cc3C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CC(CCCC)CCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8F)C7=C(C#N)C#N)sc6c5n(CC(CC)CCC	D18	16.82

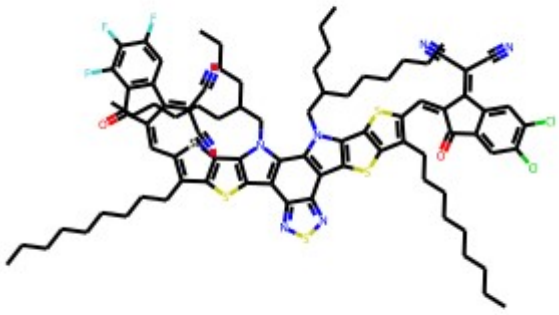
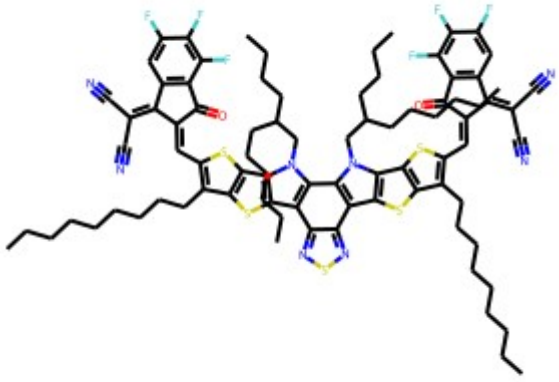
	C)c4c3n(CC(CC)CCCC)c21		
4	 C CCCCCCCCc1c(C=C2C(=O)c3c(cc(F)c(F)c3F)C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCC)c(C=C7C(=O)c8c(ccc(C)c8Br)C7=C(C#N)C#N)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	PM6	16.73
5	 C CCCCCCCCc1c(C=C2C(=O)c3c(cc(F)c(F)c3F)C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCC)c(C=C7C(=O)c8cc(Br)c(C)cc8C7	PM6	16.73

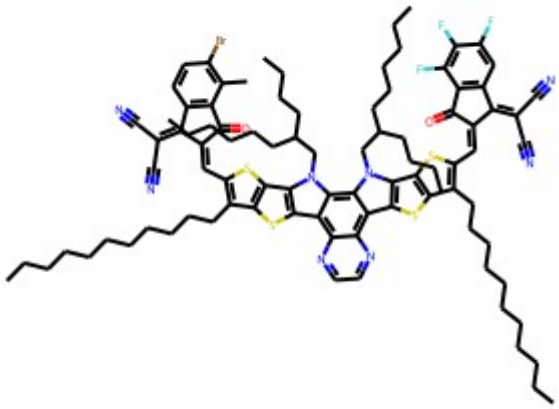
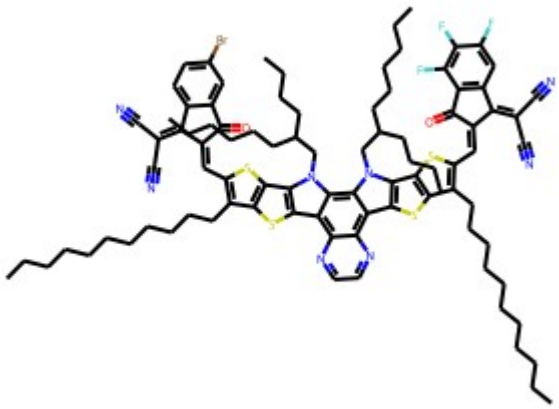
	=C(C#N)C#N)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21		
6	 C CCCCCCCCc1c(C=C2C(=O)c3c(cc(F)c(F)c3F)C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCC)c(C=C7C(=O)c8cc(Br)ccc8C7=C(C#N)C#N)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	PM6	16.73
7	 C CCCCCCCCc1c(C=C2C(=O)c3c(cc(F)c(F)c3F)C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(C	PM6	16.73

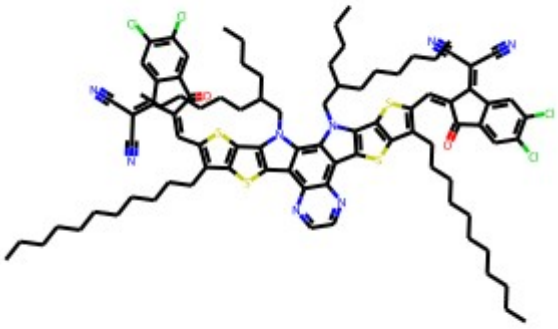
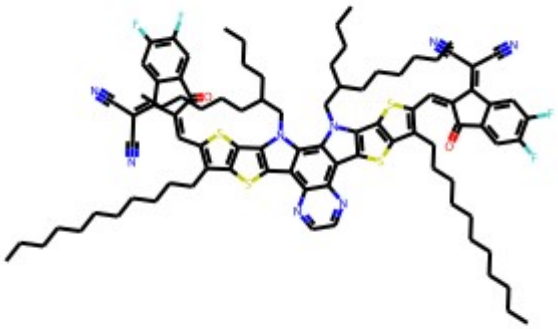
	CCCCCCCC)c(C=C7C(=O)c8ccc(F)cc8C7=C(C#N)C#N)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21		
8	 C CCCCCCCCc1c(C=C2C(=O)c3c(ccc(Br)c3C)C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8F)C7=C(C#N)C#N)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	PM6	16.73
9	 C CCCCCCCCc1c(C=C2C(=O)c3cc(Cl)c(Cl)cc3C	D18	16.71

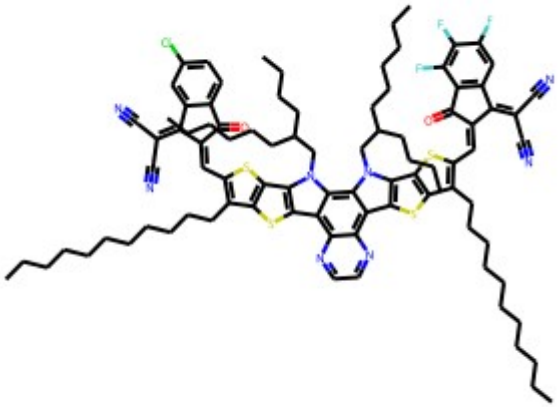
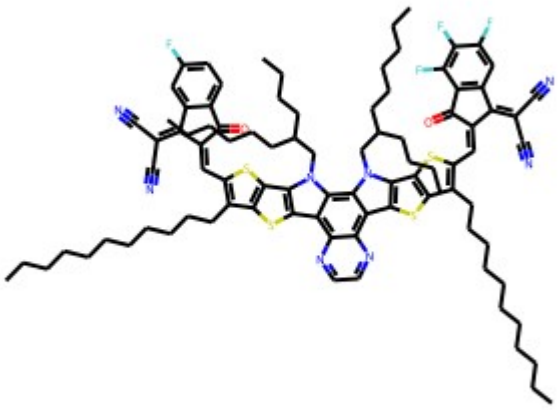
	2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCC)c(C=C7C(=O)c8cc(Cl)c(Cl)cc8C7=C(C#N)C#N)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21		
10	 C CCCCCCCCc1c(C=C2C(=O)c3cc(F)c(F)cc3C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCC)c(C=C7C(=O)c8cc(F)c(F)cc8C7=C(C#N)C#N)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	16.68
11	 C	D18	16.68

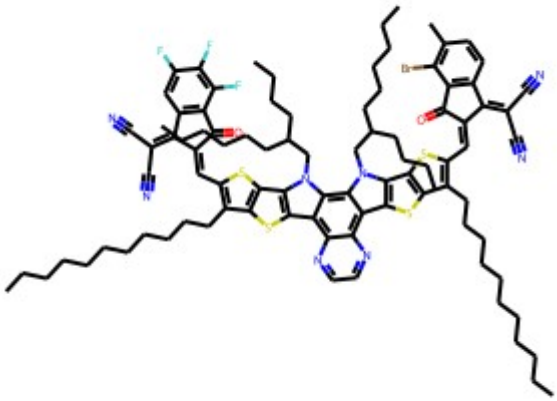
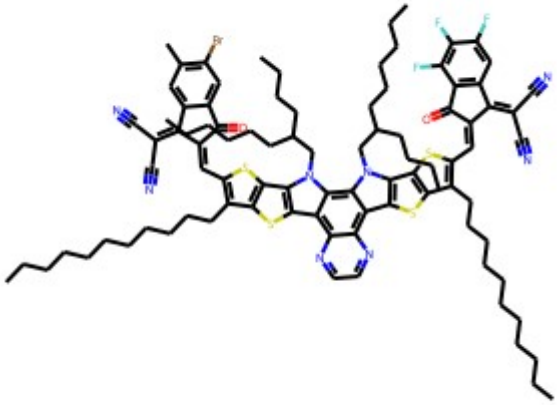
	CCCCCC(CCCC)Cc1c(C=C2C(=O)c3cc(Cl)c(Cl)cc3C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CC(CCCC)CCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8F)C7=C(C#N)C#N)sc6c5n(CC(CC)CCCC)c4c3n(CC(CC)CCCC)c21		
12	 CCCCCCCCCCCc1c(C=C2C(=O)c3c(ccc(Br)c3C)C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8F)C7=C(C#N)C#N)sc6c5n(CC(CC)CCCC)c4c3n(CC(CC)CCCC)c21	D18	16.67

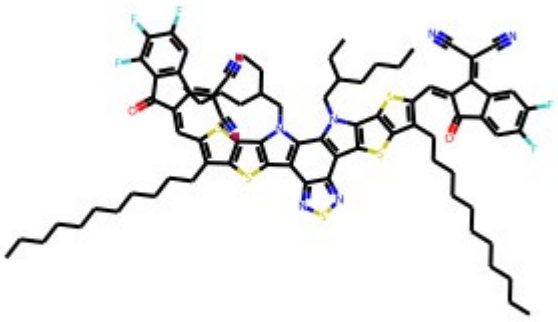
13	 C CCCCCCCCc1c(C=C2C(=O)c3cc(Cl)c(Cl)cc3C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8F)C7=C(C#N)C#N)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	16.67
14	 C CCCCCCCCc1c(C=C2C(=O)c3c(cc(F)c(F)c3F)C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8F)C7=C(C#N)C#N)sc6c5n(CC(CCCC)CCCCCC)c4	D18	16.67

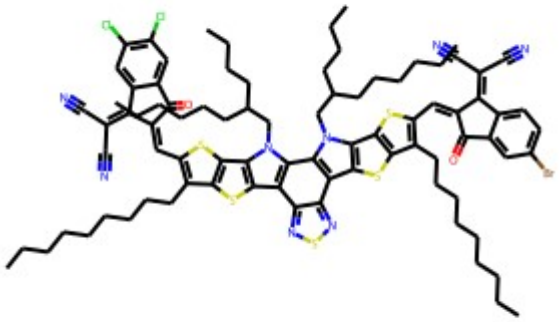
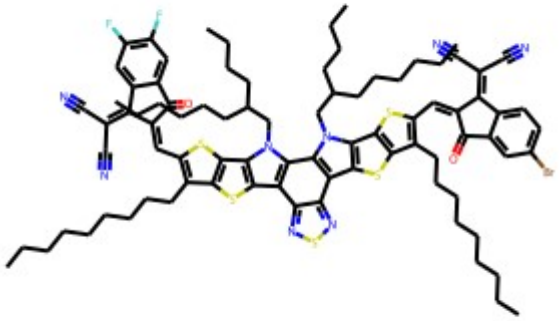
	c3n(CC(CCCC)CCCCCC)c21		
15	 CCCCCCCCCCCc1c(C=C2C(=O)c3c(ccc(Br)c3C)C2=C(C#N)C#N)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8F)C7=C(C#N)C#N)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	16.67
16	 CCCCCCCCCCCc1c(C=C2C(=O)c3cc(Br)ccc3C2=C(C#N)C#N)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8	D18	16.67

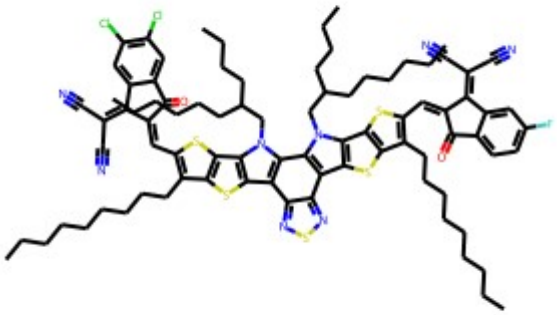
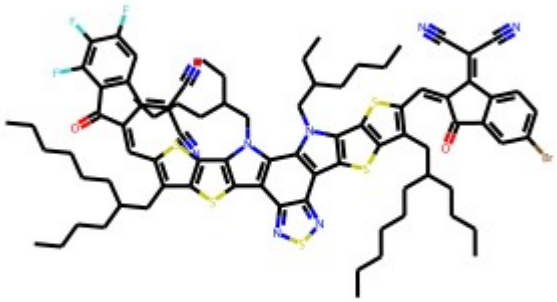
	F)C7=C(C#N)C#N)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21		
17	 CCCCCCCCCCc1c(C=C2C(=O)c3cc(Cl)c(Cl)cc3C2=C(C#N)C#N)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCCC)c(C=C7C(=O)c8cc(Cl)c(Cl)cc8C7=C(C#N)C#N)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	16.67
18	 CCCCCCCCCCc1c(C=C2C(=O)c3cc(F)c(F)cc3C2=C(C#N)C#N)sc2c1sc1c3c4nccnc4c4c5sc6c(	D18	16.67

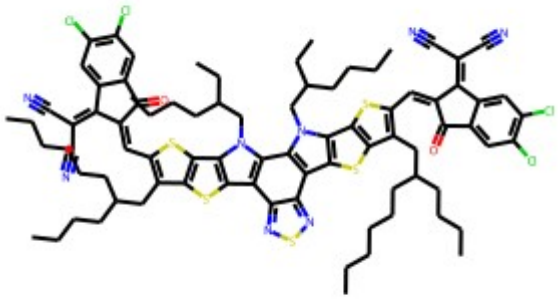
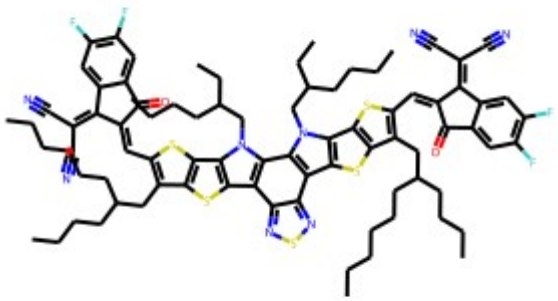
	CCCCCCCCCCC)c(C=C7C(=O)c8cc(F)c(F)cc8C7=C(C#N)C#N)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21		
19	 C CCCCCCCCCCc1c(C=C2C(=O)c3ccc(Cl)cc3C2=C(C#N)C#N)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8F)C7=C(C#N)C#N)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	16.62
20	 C CCCCCCCCCCc1c(C=C2C(=O)c3ccc(F)cc3C2	D18	16.60

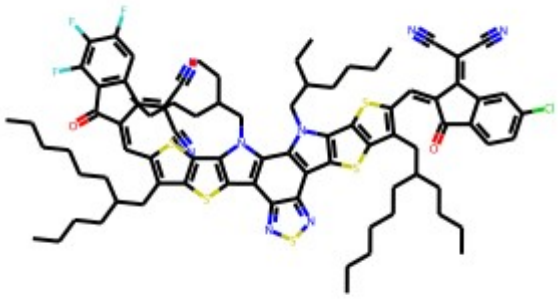
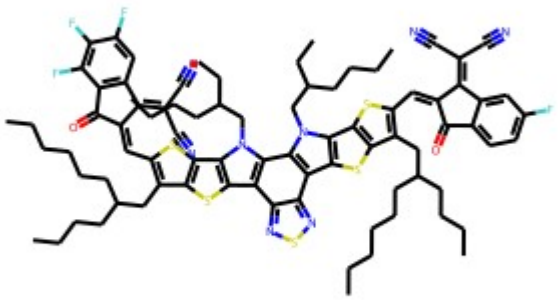
	=C(C#N)C#N)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8F)C7=C(C#N)C#N)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21		
21	 C CCCCCCCCCCc1c(C=C2C(=O)c3c(cc(F)c(F)c3F)C2=C(C#N)C#N)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCCC)c(C=C7C(=O)c8c(ccc(C)c8Br)C7=C(C#N)C#N)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	16.60
22	 C	D18	16.40

	CCCCCCCCCCc1c(C=C2C(=O)c3cc(Br)c(C)cc3C2=C(C#N)C#N)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8F)C7=C(C#N)C#N)sc6c5n(CC(CCCC)CCCCC)c4c3n(CC(CCCC)CCCCCC)c21		
23	 C CCCCCCCCCCc1c(C=C2C(=O)c3cc(F)c(F)cc3C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8F)C7=C(C#N)C#N)sc6c5n(CC(CC)CCCC)c4c3n(CC(CC)CCCC)c21	D18	16.40

24	 C CCCCCCCCc1c(C=C2C(=O)c3cc(Br)ccc3C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(C=C7C(=O)c8cc(Cl)c(Cl)cc8C7=C(C#N)C#N)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	16.40
25	 C CCCCCCCCc1c(C=C2C(=O)c3cc(Br)ccc3C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(C=C7C(=O)c8cc(F)c(F)cc8C7=C(C#N)C#N)sc6c5n(CC(CCCC)CCCCCC)c4c3n(C	D18	16.40

	C(CCCC)CCCCCC)c21		
26	 C CCCCCCCCc1c(C=C2C(=O)c3ccc(F)cc3C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(C=C7C(=O)c8cc(Cl)c(Cl)cc8C7=C(C#N)C#N)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	16.40
27	 C CCCCCC(CCCC)Cc1c(C=C2C(=O)c3cc(Br)ccc3C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CC(CCCC)CCCCCC)c(C=C7C(=O)c8c(cc(F)c(	D18	16.40

	F)c8F)C7=C(C#N)C#N)sc6c5n(CC(CC)CCCC)c4c3n(CC(CC)CCCC)c21		
28	 C CCCCCC(CCCC)Cc1c(C=C2C(=O)c3cc(Cl)c(Cl)cc3C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CC(CCCC)CCCCCC)c(C=C7C(=O)c8cc(Cl)c(Cl)cc8C7=C(C#N)C#N)sc6c5n(CC(CC)CCCC)c4c3n(CC(CC)CCCC)c21	D18	16.39
29	 C CCCCCC(CCCC)Cc1c(C=C2C(=O)c3cc(F)c(F)cc3C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6	D18	16.39

	c(CC(CCCC)CCCCCC)c(C=C7C(=O)c8cc(F)c(F)cc8C7=C(C#N)C#N)sc6c5n(CC(CC)CCCC)c4c3n(CC(CC)CCCC)c21		
30	 C CCCCCC(CCCC)Cc1c(C=C2C(=O)c3ccc(Cl)cc3C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CC(CCCC)CCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8F)C7=C(C#N)C#N)sc6c5n(CC(CC)CCCC)c4c3n(CC(CC)CCCC)c21	D18	16.30
31	 C CCCCCC(CCCC)Cc1c(C=C2C(=O)c3ccc(F)cc3	D18	16.30

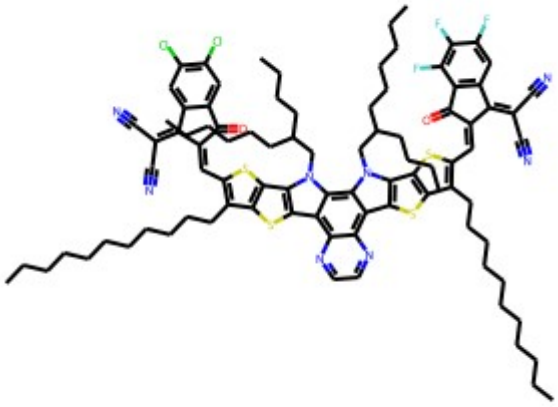
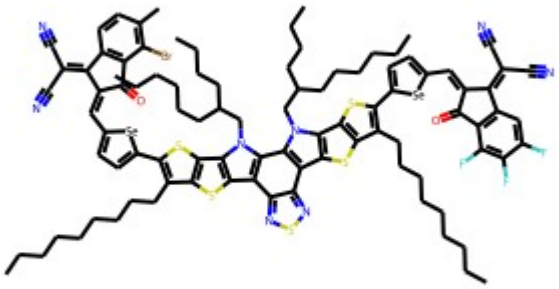
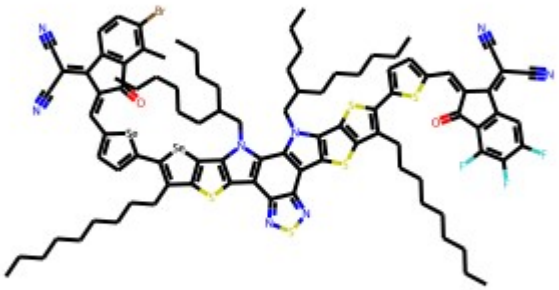
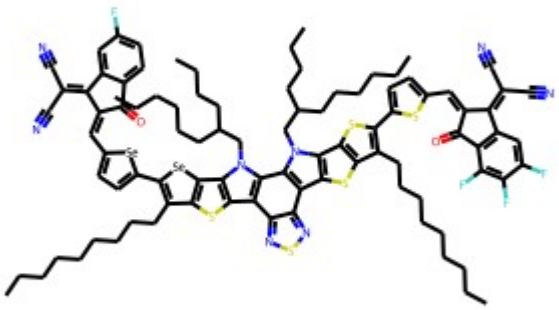
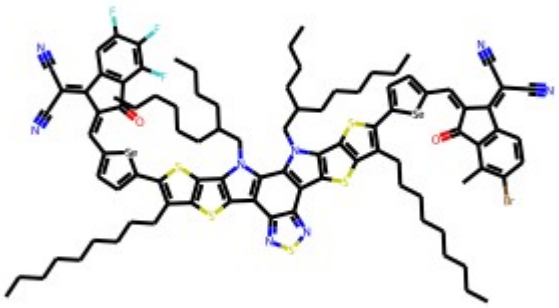
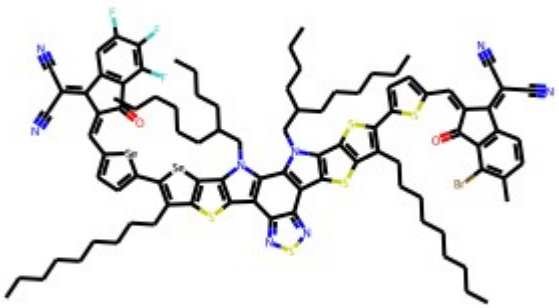
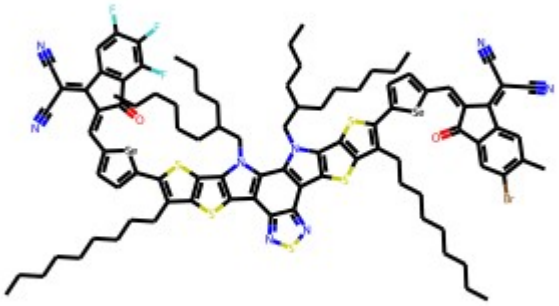
	C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CC(CCCC)CCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8F)C7=C(C#N)C#N)sc6c5n(CC(CC)CCCC)c4c3n(CC(CC)CCCC)c21		
32	 CCCCCCCCCCc1c(C=C2C(=O)c3cc(Cl)c(Cl)cc3C2=C(C#N)C#N)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8F)C7=C(C#N)C#N)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	16.30

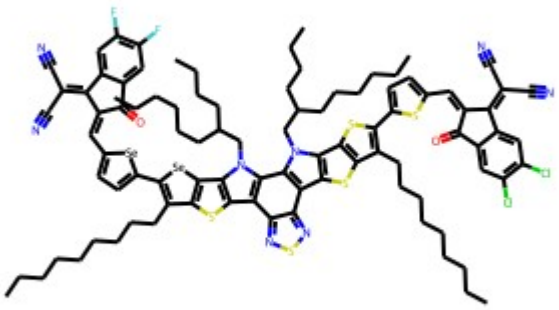
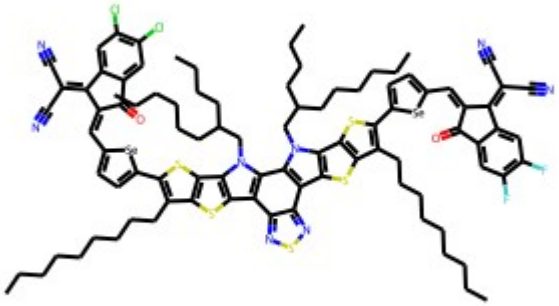
Table S12 The 32 A_1-π_1-D-π_2-A_2 type acceptor molecules with the higher PCE in the 100th generation.

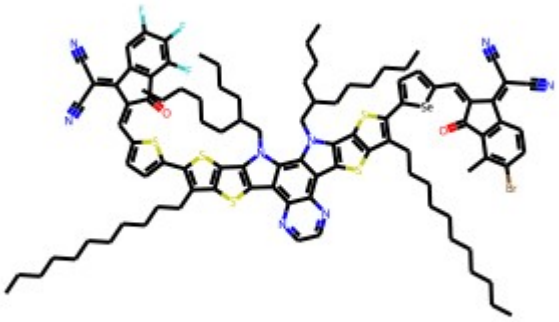
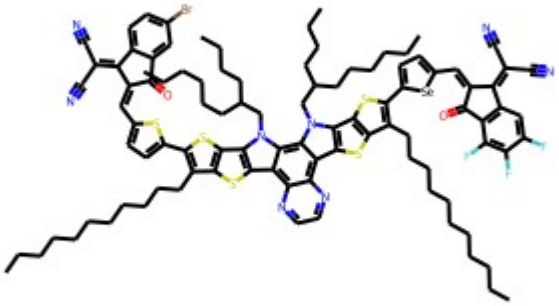
serial number	Designed acceptor molecule	Donor molecule	PCE Prediction

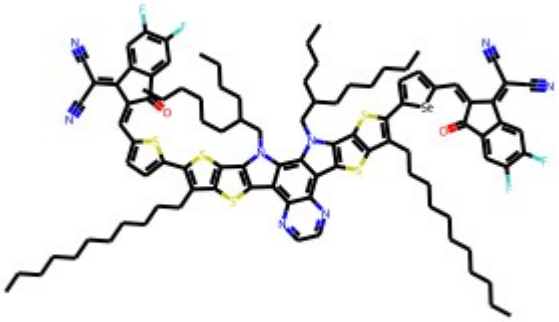
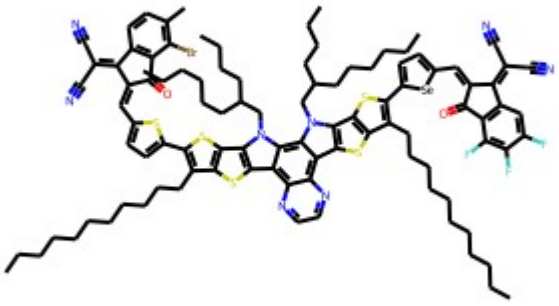
1	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(cc(F)c(F)c4F)C3=C(C#N)C#N)[se]2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(ccc(C)c9Br)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.39741
2	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(cc(F)c(F)c4F)C3=C(C#N)C#N)s2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(ccc(Br)c9C)C8=C(C#N)C#N)[se]7)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.39741

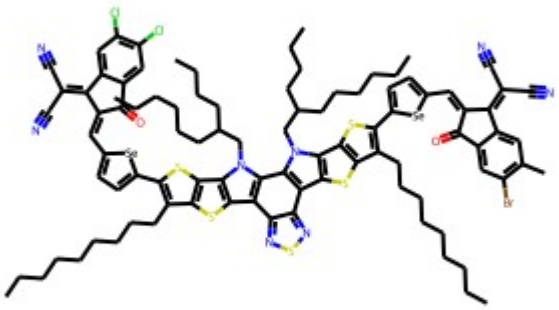
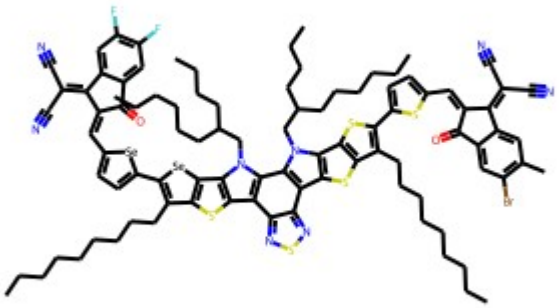
3	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(cc(F)c(F)c4F)C3=C(C#N)C#N)s2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7ccc(C=C8C(=O)c9ccc(F)cc9C8=C(C#N)C#N)[se]7)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.39741
4	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(ccc(Br)c4C)C3=C(C#N)C#N)[se]2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(cc(F)c(F)c9F)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.39741

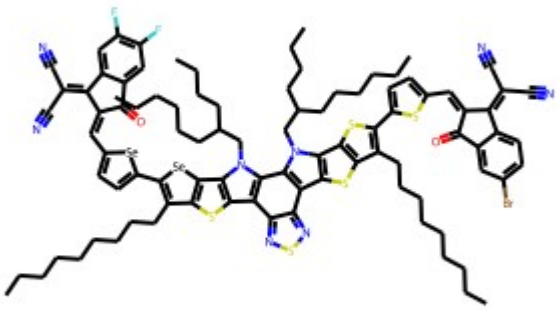
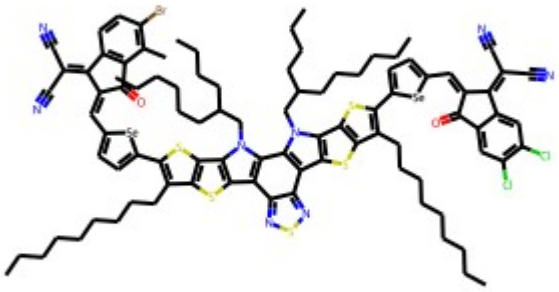
5	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(ccc(C)c4Br)C3=C(C#N)C#N)s2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(cc(F)c(F)c9F)C8=C(C#N)C#N)[se]7)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.39741
6	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(Br)c(C)cc4C3=C(C#N)C#N)[se]2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(cc(F)c(F)c9F)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.39741

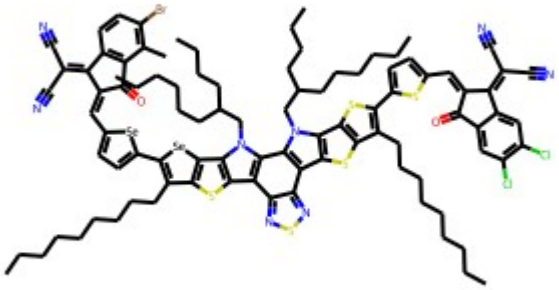
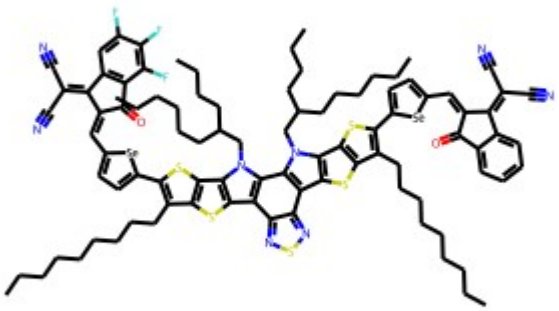
7	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(Cl)c(Cl)cc4C3=C(C#N)C#N)s2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7ccc(C=C8C(=O)c9cc(F)c(F)cc9C8=C(C#N)C#N)[se]7)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.39741
8	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(F)c(F)cc4C3=C(C#N)C#N)[se]2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7ccc(C=C8C(=O)c9cc(Cl)c(Cl)cc9C8=C(C#N)C#N)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.39741

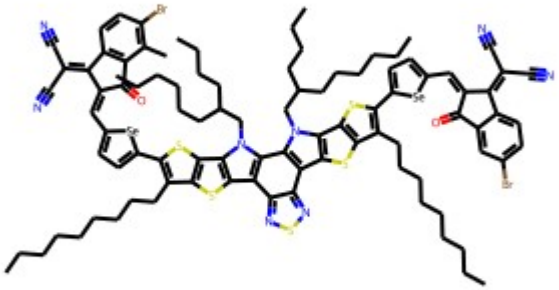
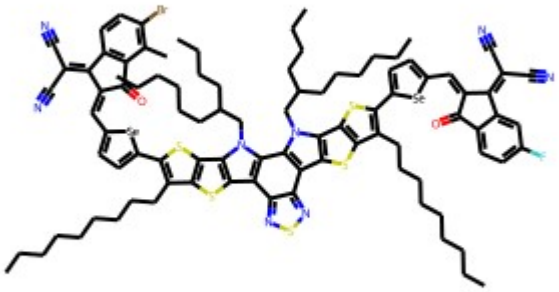
9	 CCCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(cc(F)c(F)c4F)C3=C(C#N)C#N)s2)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(ccc(Br)c9C)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.31573
10	 CCCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(Br)ccc4C3=C(C#N)C#N)s2)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(cc(F)c(F)c9F)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.31573

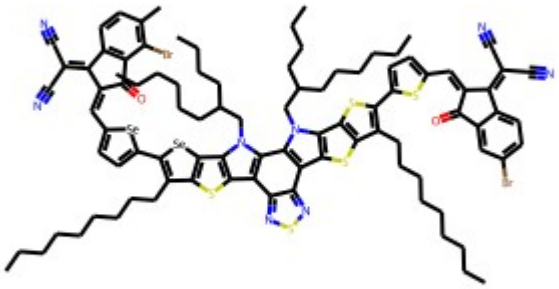
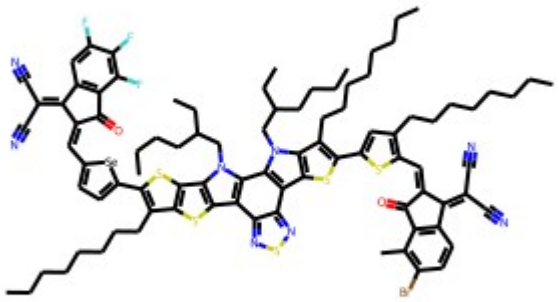
11	 CCCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(F)c(F)cc4C3=C(C#N)C#N)s2)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9cc(F)c(F)cc9C8=C(C#N)C#N)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.31573
12	 CCCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(ccc(C)c4Br)C3=C(C#N)C#N)s2)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(cc(F)c(F)c9F)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.30564

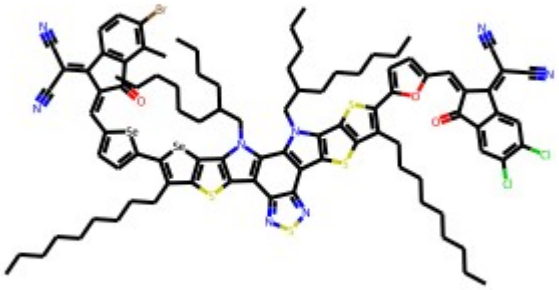
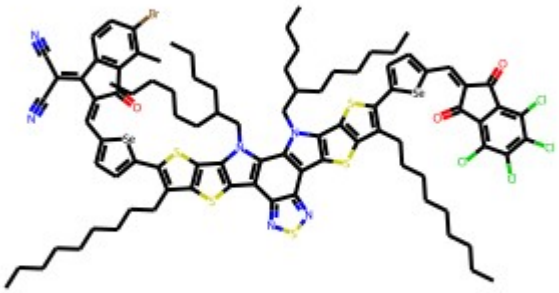
13	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(Br)c(C)cc4C3=C(C#N)C#N)[se]2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9cc(Cl)c(Cl)cc9C8=C(C#N)C#N)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.27006
14	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(Br)c(C)cc4C3=C(C#N)C#N)s2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9cc(F)c(F)cc9C8=C(C#N)C#N)[se]7)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.27006

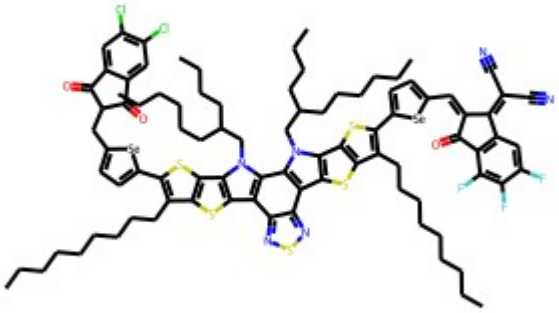
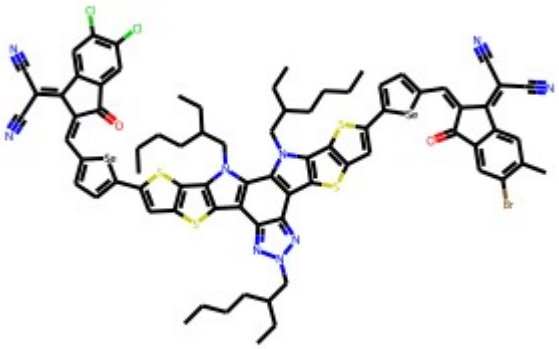
15	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(Br)ccc4C3=C(C#N)C#N)s2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7ccc(C=C8C(=O)c9cc(F)c(F)cc9C8=C(C#N)C#N)[se]7)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.27006
16	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(Cl)c(Cl)cc4C3=C(C#N)C#N)[se]2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(ccc(Br)c9C)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.27006

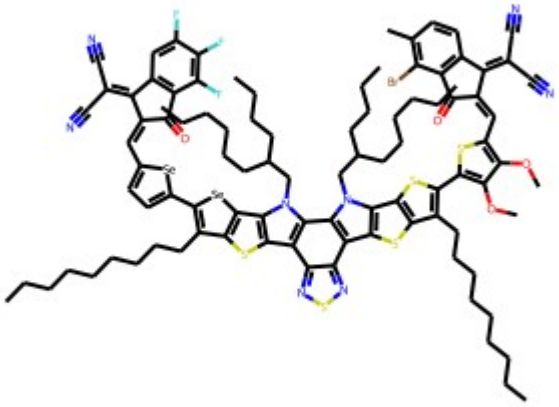
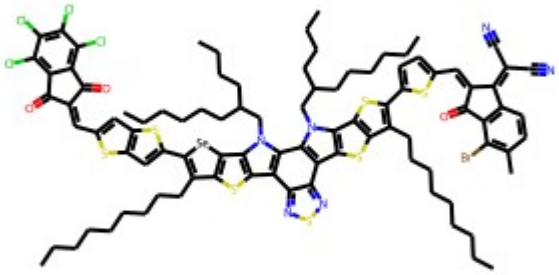
17	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(Cl)c(Cl)cc4C3=C(C#N)C#N)s2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(ccc(Br)c9C)C8=C(C#N)C#N)[se]7)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.27006
18	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4ccccc4C3=C(C#N)C#N)[se]2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(cc(F)c(F)c9F)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.27006

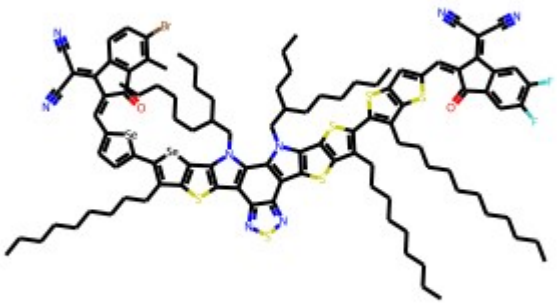
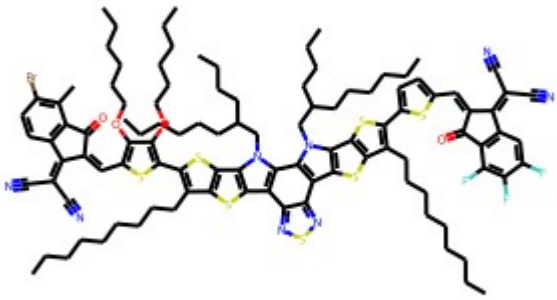
19	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(Br)ccc4C3=C(C#N)C#N)[se]2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(ccc(Br)c9C)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.25616
20	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4ccc(F)cc4C3=C(C#N)C#N)[se]2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(ccc(Br)c9C)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.25616

21	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(Br)ccc4C3=C(C#N)C#N)s2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(ccc(C)c9Br)C8=C(C#N)C#N)[se]7)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	15.24683
22	 CCCCCCCCCc1cc(-c2sc3c4c5nsnc5c5c6sc7c(CCCCCCCC)c(-c8ccc(C=C9C(=O)c%10c(cc(F)c(F)c%10F)C9=C(C#N)C#N)[se]8)sc7c6n(CC(CC)CCCC)c5c4n(CC(CC)CCCC)c3c2CCCCCCCC)sc1C=C1C(=O)c2c(ccc(Br)c2C)C1=C(C#N)C#N	D18	15.08435

23	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(Cl)c(Cl)cc4C3=C(C#N)C#N)o2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(ccc(Br)c9C)C8=C(C#N)C#N)[se]7)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	14.97725
24	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(Cl)c(Cl)c(Cl)c(Cl)c4C3=O)[se]2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(ccc(Br)c9C)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	14.70154

25	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(cc(F)c(F)c4F)C3=C(C#N)C#N)[se]2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7ccc(CC8C(=O)c9cc(Cl)c(Cl)cc9C8=O)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	14.37744
26	 CCCCC(CC)Cn1nc2c(n1)c1c3sc4cc(-c5ccc(C=C6C(=O)c7cc(Cl)c(Cl)cc7C6=C(C#N)C#N)[se]5)sc4c3n(CC(CC)CCCC)c1c1c2c2sc3cc(-c4ccc(C=C5C(=O)c6cc(Br)c(C)cc6C5=C(C#N)C#N)[se]4)sc3c2n1CC(CC)CCCC	D18	14.3408

27	 CCCCCCCCCCc1c(-c2sc(C=C3C(=O)c4c(ccc(C)c4Br)C3=C(C#N)C#N)c(OC)c2OC)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(cc(F)c(F)c9F)C8=C(C#N)C#N)[se]7)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	14.14332
28	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(ccc(C)c4Br)C3=C(C#N)C#N)s2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7cc8sc(C=C9C(=O)c%10c(Cl)c(Cl)c(Cl)c(Cl)c%10C9=O)cc8s7)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	13.51567

29	 CCCCCCCCCCCc1c(-c2sc3c(sc4c5c6nsnc6c6c7sc8c(CCCCCCCCC)c(-c9ccc(C=C%10C(=O)c%11c(ccc(Br)c%11C)C%10=C(C#N)C#N)[se]9)[se]c8c7n(CC(CCCC)CCCCCC)c6c5n(CC(CCCC)CCCCCC)c34)c2CCCCCCCCC)sc2cc(C=C3C(=O)c4cc(F)c(F)cc4C3=C(C#N)C#N)sc12	D18	13.34386
30	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(cc(F)c(F)c4F)C3=C(C#N)C#N)s2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCC)c(-c7sc(C=C8C(=O)c9c(ccc(Br)c9C)C8=C(C#N)C#N)c(OCCCCCC)c7OCCCCCC)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	13.25576

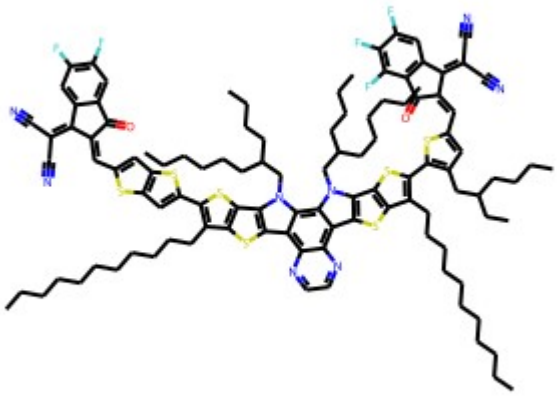
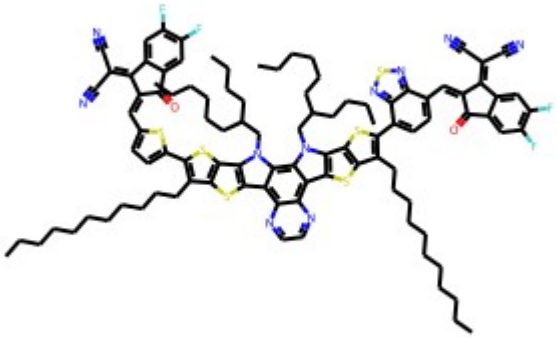
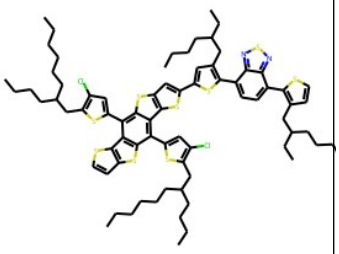
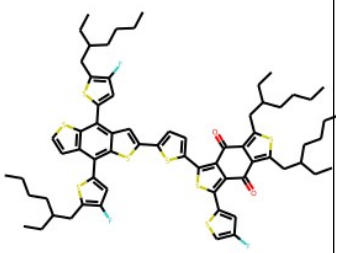
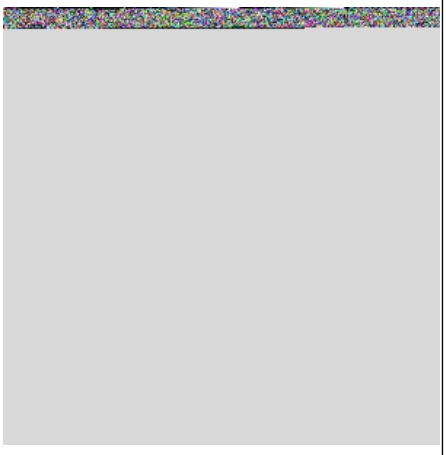
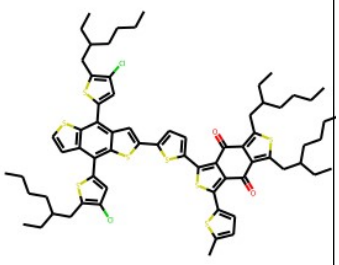
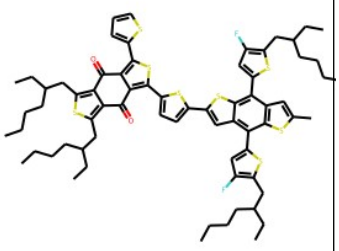
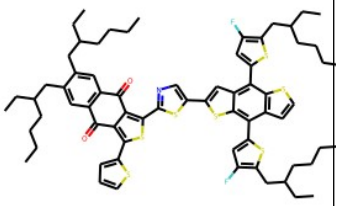
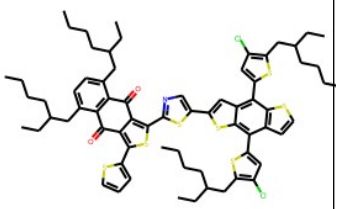
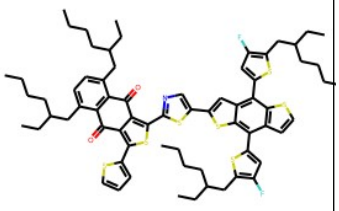
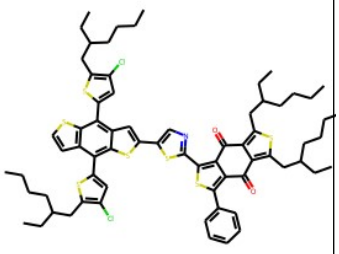
31	 CCCCCCCCCCCc1c(-c2cc3sc(C=C4C(=O)c5cc(F)c(F)cc5C4=C(C#N)C#N)cc3s2)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCCC)c(-c7sc(C=C8C(=O)c9c(cc(F)c(F)c9F)C8=C(C#N)C#N)cc7CC(CC)CCCC)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	13.18019
32	 CCCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(F)c(F)cc4C3=C(C#N)C#N)s2)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9cc(F)c(F)cc9C8=C(C#N)C#N)c8nsnc78)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	D18	12.93861

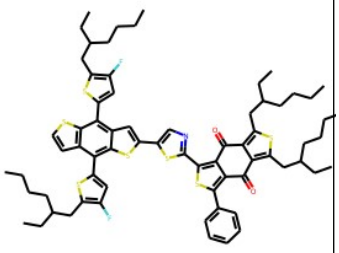
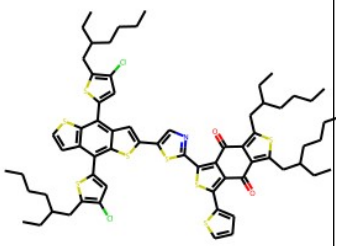
Table S13: Among the 32 donor - acceptor pairs with the highest PCE in the 100th generation, after deleting the existing ones, the remaining 30 new donor - acceptor pairs of the A_1-D-A_2 type.

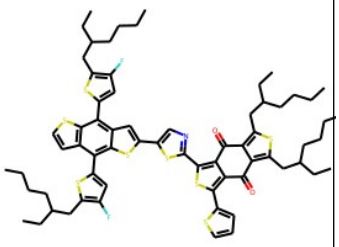
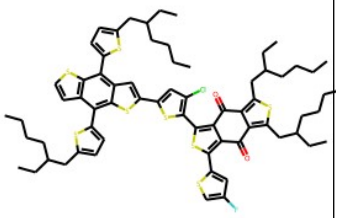
serial number	Donor molecule	Acceptor molecule	PCE Prediction
1	 CCCCCCC(CCCC)Cc1sc(-c2c3sc4cc(-c5cc(CC(CC)CCCC)c(-c6ccc(-c7sccc7CC(CC)CCCC)c7nsnc67)s5)sc4c3c(-c3cc(Cl)c(CC(CCCC)CCCCCC)s3)c3sc4ccsc4c23)cc1Cl	 CCCCCCCCCCCc1c(C=C2C(=O)c3c(ccc(Br)c3C)C2=C(C#N)C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8F)C7=C(C#N)C#N)sc6c5n(CC(CC)CCCC)c4c3n(CC(CC)CCCC)c21	16.85495
2	 CCCCC(CC)Cc1sc(-c2c3cc(-c4ccc(-c5sc(-c6cc(F)cs6)c6c5C(=O)c5	 CCCCCCC(CCCC)Cc1c(C=C2C(=O)c3cc(Br)ccc3C2=C(C#N)	16.70728

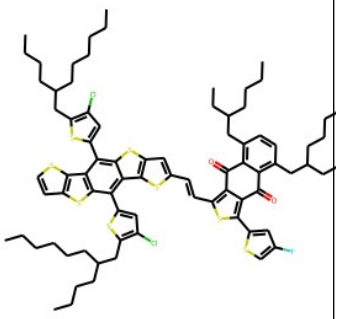
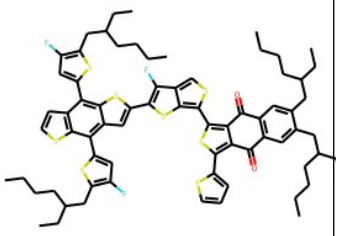
	c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(F)c(CC(CC)CCCC)s3)c3ccsc23)cc1F		
3	 CCCCC(CC)Cc1sc(-c2c3cc(-c4ccc(-c5sc(-c6ccc(C)s6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(Cl)c(CC(CC)CCCC)s3)c3ccsc23)cc1Cl	C#N)sc2c1sc1c3c4nsnc4c4c5sc6c(CC(CCCC)CCCCCC)c(C=C7C(=O)c8c(cc(F)c(F)c8F)C7=C(C#N)C#N)sc6c5n(CC(CC)CCCC)c4c3n(CC(CC)CCCC)c21	16.70728
4	 CCCCC(CC)Cc1sc(-c2c3cc(-c4ccc(-c5sc(-c6cccs6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(C		16.70728

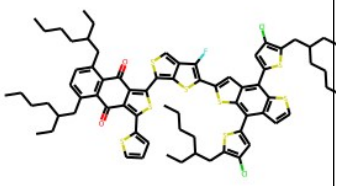
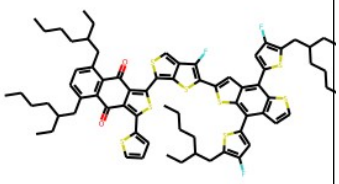
	C)CCCC)c5C6=O)s4)sc3c(-c3cc(F)c(CC(CC)CCCC)s3)c3cc(C)sc23)cc1F		
5	 CCCCC(CC)Cc1cc2c(cc1CC(CC)CCCC)C(=O)c1c(-c3ncc(-c4cc5c(-c6cc(F)c(CC(CC)CCCC)s6)c6sccc6c(-c6cc(F)c(CC(CC)CCCC)s6)c5s4)s3)sc(-c3cccs3)c1C2=O		16.69299
6	 CCCCC(CC)Cc1ccc(CC(CC)CCCC)c2c1C(=O)c1c(-c3cccs3)sc(-c3ncc(-c4cc5c(-c6cc(Cl)c(CC(CC)CCCC		16.69299

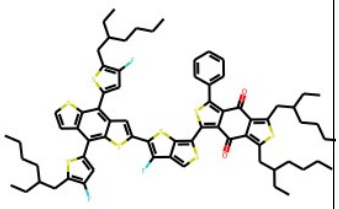
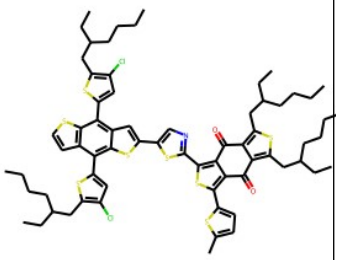
	)s6)c6sccc6c(-c6cc(Cl)c(CC(CC)CCCC)s6)c5s4)s3)c1C2=O		
7	 CCCCC(CC)Cc1ccc(CC(CC)CCCC)c2c1C(=O)c1c(-c3cccs3)sc(-c3ncc(-c4cc5c(-c6cc(F)c(CC(CC)CCCC)s6)c6sccc6c(-c6cc(F)c(CC(CC)CCCC)s6)c5s4)s3)c1C2=O		16.69299
8	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cnc(-c5sc(-c6ccccc6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-		16.69299

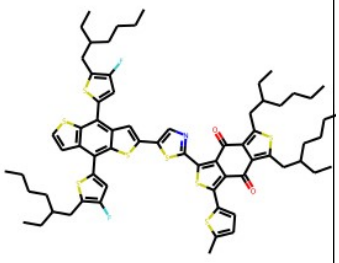
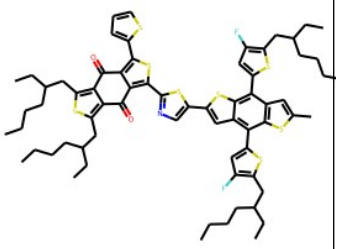
	c3cc(Cl)c(CC(CC)CCCC)s3)c3ccsc23)cc1Cl		
9	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cnc(-c5sc(-c6ccccc6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(F)c(CC(CC)CCCC)s3)c3ccsc23)cc1F		16.69299
10	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cnc(-c5sc(-c6cccs6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(Cl)c(CC(CC)CCCC		16.69299

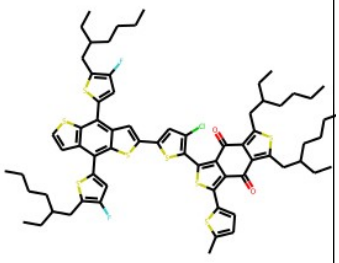
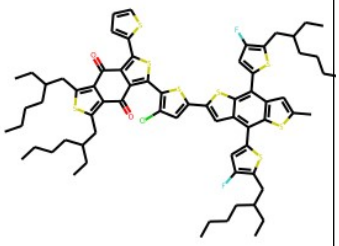
	)s3)c3ccsc23)cc1Cl		
11	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cnc(-c5sc(-c6cccs6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(F)c(CC(CC)CCCC)s3)c3ccsc23)cc1F		16.6289
12	 CCCCC(CC)Cc1ccc(-c2c3cc(-c4cc(Cl)c(-c5sc(-c6cc(F)cs6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3ccc(CC(CC)CCCC)s3)		16.6289

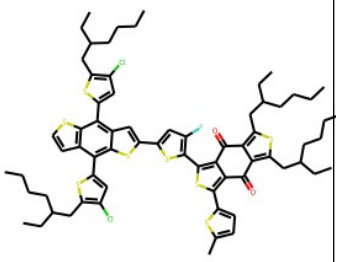
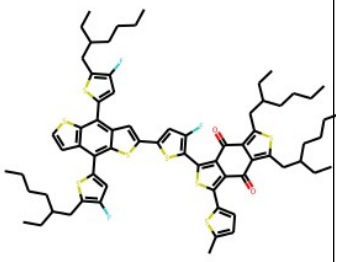
	c3ccsc23)s1		
13	 CCCCCCC(CCCC)Cc1sc(-c2c3sc4cc(C=Cc5sc(-c6cc(F)cs6)c6c5C(=O)c5c(CC(CC)CCCC)ccc(CC(CC)CCCC)c5C6=O)sc4c3c(-c3cc(Cl)c(CC(CCCC)CCCCCC)s3)c3sc4ccsc4c23)cc1Cl		16.31325
14	 CCCCC(CC)Cc1cc2c(cc1CC(CC)CCCC)C(=O)c1c(-c3scc4c(F)c(-c5cc6c(-c7cc(F)c(CC(CC)CCCC)s7)c7sccc7c(-c7cc(F)c(CC(CC)CCCC)		16.31325

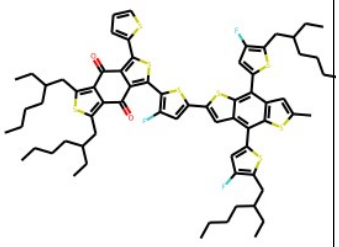
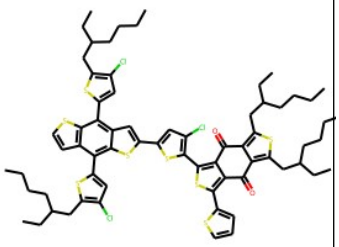
	s7)c6s5)sc34)sc(-c3cccs3)c1C2=O		
15	 CCCCC(CC)Cc1ccc(CC(CC)CCCC)c2c1C(=O)c1c(-c3cccs3)sc(-c3scc4c(F)c(-c5cc6c(-c7cc(Cl)c(CC(CC)CCCC)s7)c7sccc7c(-c7cc(Cl)c(CC(CC)CCCC)s7)c6s5)sc34)c1C2=O		16.31325
16	 CCCCC(CC)Cc1ccc(CC(CC)CCCC)c2c1C(=O)c1c(-c3cccs3)sc(-c3scc4c(F)c(-c5cc6c(-c7cc(F)c(CC(CC)CCCC)s7)c7sccc7c(-c7cc(F)c(CC(CC)CCCC)		16.31325

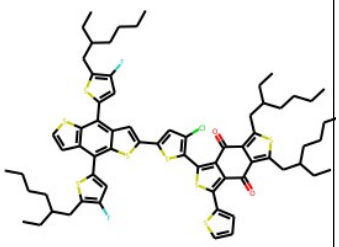
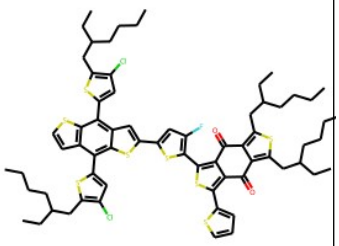
	s7)c6s5)sc34)c1C2=O		
17	 CCCCC(CC)Cc1sc(-c2c3cc(-c4sc5c(-c6sc(-c7ccccc7)c7c6C(=O)c6c(CC(CC)CCCC)sc(CC(CC)CCCC)c6C7=O)scc5c4F)sc3c(-c3cc(F)c(CC(CC)CCCC)s3)c3ccsc23)cc1F		16.31325
18	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cnc(-c5sc(-c6ccc(C)s6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(Cl)c(CC(CC)CCCC)s3)c3ccsc23)cc1Cl		16.28141

19	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cnc(-c5sc(-c6ccc(C)s6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(F)c(CC(CC)CCCC)s3)c3ccsc23)cc1F		16.28141
20	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cnc(-c5sc(-c6cccs6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(F)c(CC(CC)CCCC)s3)c3cc(C)sc23)cc1F		16.25663

21	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cc(Cl)c(-c5sc(-c6ccc(C)s6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(F)c(CC(CC)CCCC)s3)c3ccsc23)cc1F		16.23751
22	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cc(Cl)c(-c5sc(-c6cccs6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(F)c(CC(CC)CCCC)		16.23751

	s3)c3cc(C)sc23)cc1F		
23	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cc(F)c(-c5sc(-c6ccc(C)s6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(Cl)c(CC(CC)CCCC)s3)c3ccsc23)cc1Cl		16.23751
24	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cc(F)c(-c5sc(-c6ccc(C)s6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(F)c(CC(CC)CCCC)s3)c3ccsc23)cc1F		16.22315

25	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cc(F)c(-c5sc(-c6cccs6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(F)c(CC(CC)CCCC)s3)c3cc(C)sc23)cc1F		16.22315
26	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cc(Cl)c(-c5sc(-c6cccs6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(Cl)c(CC(CC)CCCC)s3)c3ccsc23)cc1Cl		16.20962

27	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cc(Cl)c(-c5sc(-c6cccs6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(F)c(CC(CC)CCCC)s3)c3ccsc23)cc1F		16.20962
28	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cc(F)c(-c5sc(-c6cccs6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(Cl)c(CC(CC)CCCC)s3)c3ccsc23)cc1Cl		16.20962

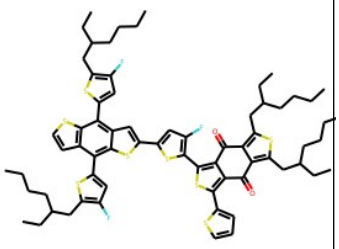
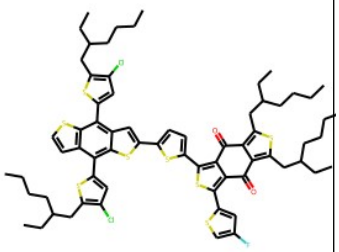
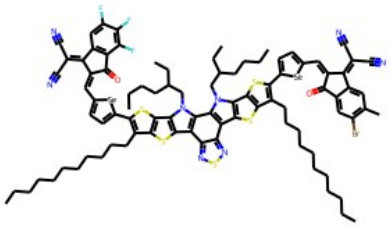
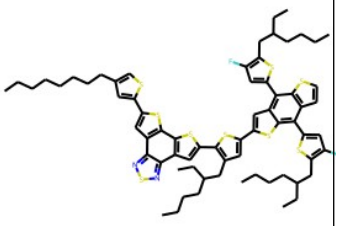
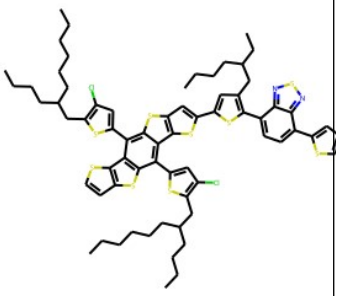
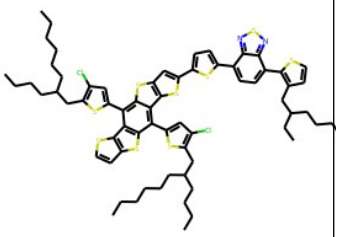
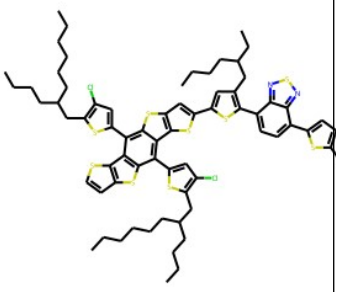
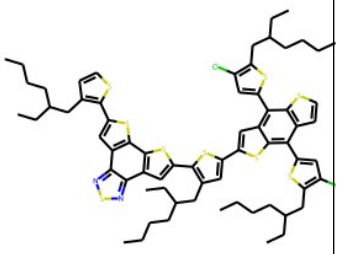
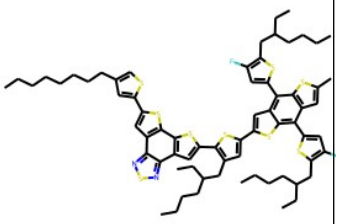
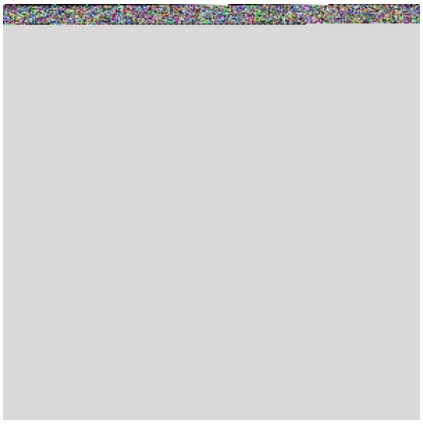
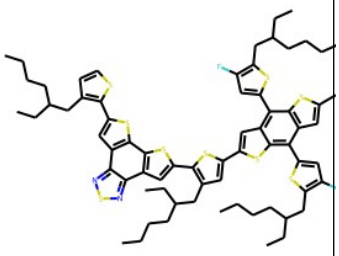
29	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cc(F)c(-c5sc(-c6cccs6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(F)c(CC(CC)CCCC)s3)c3ccsc23)cc1F		16.20962
30	 CCCCC(CC)Cc1sc(-c2c3cc(-c4ccc(-c5sc(-c6cc(F)cs6)c6c5C(=O)c5c(CC(CC)CCCC)sc(CC(CC)CCCC)c5C6=O)s4)sc3c(-c3cc(Cl)c(CC(CC)CCCC)s3)c3ccsc23)cc1Cl		16.20962

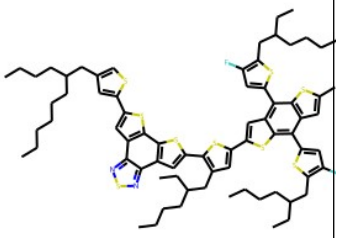
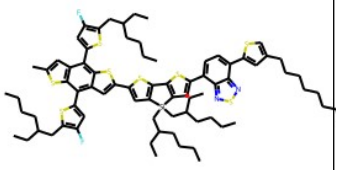
Table S14 The 32 donor - acceptor pairs of the A_1-π_1-D-π_2-A_2 type with the higher PCE in the 100th generation.

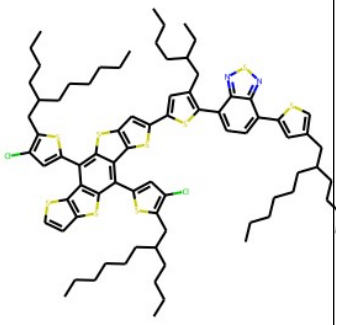
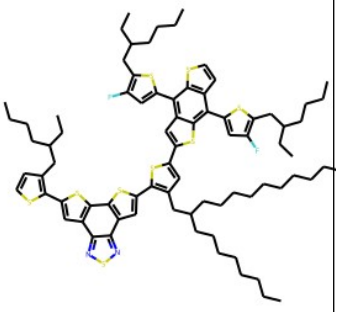
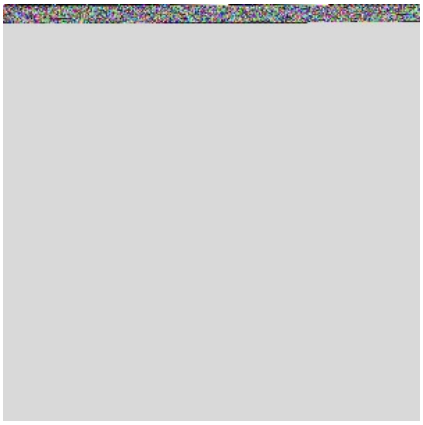
serial number	Donor molecule	Acceptor molecule	PCE Prediction
1	 CCCCCCC(CCCC)Cc1sc(-c2c3sc4cc(-c5cc(CC(CC)CCCC)c(-c6ccc(-c7sccc7CC(CC)CCCC)c7nsnc67)s5)sc4c3c(-c3cc(Cl)c(CC(CCCC)CCCCCC)s3)c3sc4ccsc4c23)cc1Cl	 CCCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(Br)c(C)cc4C3=C(C#N)C#N)[se]2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(cc(F)c(F)c9F)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CC)CCCC)c4c3n(CC(CC)CCCC)c21	15.64759
2	 CCCCCCCCCc1csc(-c2cc3c4nsnc4c4cc(-c5sc(-c6cc7c(-c8cc(F)c(CC(CC)CCCC)	 CCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(cc(F)c(F)c4F)C3=C(C#N)C#N)s2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCC	15.33859

	s8)c8sccc8c(-c8cc(F)c(CC(CC)CCCC)s8)c7s6)cc5CC(CC)CCCC)sc4c3s2)c1	CCC)c(-c7ccc(C=C8C(=O)c9c(ccc(Br)c9C)C8=C(C#N)C#N)[se]7)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	
3	 CCCCCCC(CCCC)Cc1sc(-c2c3sc4cc(-c5cc(CC(CC)CCCC)c(-c6ccc(-c7cccs7)c7nsnc67)s5)sc4c3c(-c3cc(Cl)c(CC(CCCC)CCCCCC)s3)c3sc4ccsc4c23)cc1Cl		15.30276
4	 CCCCCCC(CCCC)Cc1sc(-c2c3sc4cc(-c5ccc(-c6ccc(-c7sccc7CC(CC)CCCC)c		15.30276

	7nsnc67)s5)sc4c3c(-c3cc(Cl)c(CC(CCCC)CCCCCC)s3)c3sc4ccsc4c23)cc1Cl		
5	 CCCCCCC(CCCC)Cc1sc(-c2c3sc4cc(-c5cc(CC(CC)CCCC)c(-c6ccc(-c7ccc(C)s7)c7nsnc67)s5)sc4c3c(-c3cc(Cl)c(CC(CCCC)CCCCCC)s3)c3sc4ccsc4c23)cc1Cl		15.28914
6	 CCCCC(CC)Cc1ccsc1-c1cc2c3nsnc3c3cc(-c4sc(-c5cc6c(-c7cc(Cl)c(CC(CC)CCCC	 CCCCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(cc(F)c(F)c4F)C3=C(C#N)C#N)s2)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCCCC)c(-	15.23007

	)s7)c7sccc7c(-c7cc(Cl)c(CC(CC)CCCC)s7)c6s5)cc4CC(CC)CCCC)sc3c2s1	c7ccc(C=C8C(=O)c9c(ccc(Br)c9C)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	
7	 CCCCCCCCc1csc(-c2cc3c4nsnc4c4cc(-c5sc(-c6cc7c(-c8cc(F)c(CC(CC)CCCC)s8)c8sc(C)cc8c(-c8cc(F)c(CC(CC)CCCC)s8)c7s6)cc5CC(CC)CCCC)sc4c3s2)c1	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(cc(F)c(F)c4F)C3=C(C#N)C#N)s2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(ccc(Br)c9C)C8=C(C#N)C#N)[se]7)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	15.20528
8	 CCCCC(CC)Cc1ccsc1-c1cc2c3nsnc3c3cc(-c4sc(-c5cc6c(-c7cc(F)c(CC(CC)CCCC)s7)c7sc(C)cc7c(-		15.1974

	c7cc(F)c(CC(CC)CCCC)s7)c6s5)cc4CC(CC)CCCC)sc3c2s1		
9	 CCCCCCC(CCCC)Cc1csc(-c2cc3c4nsnc4c4cc(-c5sc(-c6cc7c(-c8cc(F)c(CC(CC)CCCC)s8)c8sc(C)cc8c(-c8cc(F)c(CC(CC)CCCC)s8)c7s6)cc5CC(CC)CCCC)sc4c3s2)c1		15.18754
10	 CCCCCCCCc1csc(-c2ccc(-c3cc4c(s3)-c3sc(-c5cc6c(-c7cc(F)c(CC(CC)CCCC)s7)c7sc(C)cc7c(-c7cc(F)c(CC(CC)CCCC)		15.00396

	s7)c6s5)cc3[Si]4(CC(CC)CCCC)CC(CC)CCCC)c3nsnc23)c1		
11	 CCCCCCC(CCCC)Cc1csc(-c2ccc(-c3sc(-c4cc5sc6c(-c7cc(Cl)c(CC(CCCC)CCCCCC)s7)c7c(sc8ccsc87)c(-c7cc(Cl)c(CC(CCCC)CCCCCC)s7)c6c5s4)cc3CC(CC)CCCC)c3nsnc23)c1		15.00357
12	 CCCCCCCCCCC(CCCCCCCC)Cc1cc(-c2cc3c(-c4cc(F)c(CC(CC)CCCC)s4)c4sccc4c(-c4cc(F)c(CC(CC)CCCC)	 CCCCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(Br)c(C)cc4C3=C(C#N)C#N)[se]2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(cc(F)c(F)	15.00025

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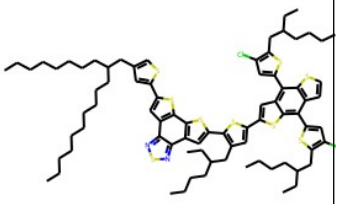
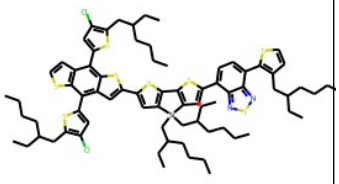
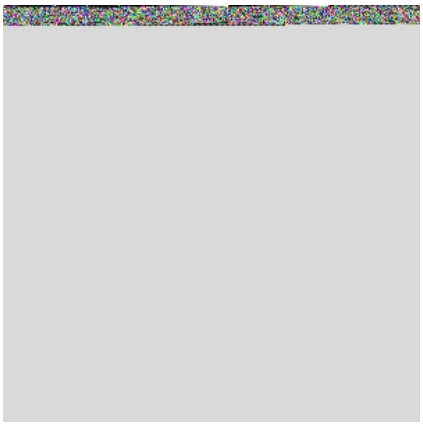
13	 CCCCCCCCCCCC(CCCCCCCCC)Cc1csc(-c2cc3c4nsnc4c4cc(-c5sc(-c6cc7c(-c8cc(Cl)c(CC(CC)CCCC)s8)c8sccc8c(-c8cc(Cl)c(CC(CC)CCCC)s8)c7s6)cc5CC(CC)CCCC)sc4c3s2)c1	c9F)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CC)CCCC)c4c3n(CC(CC)CCCC)c21	15.00025
14	 CCCCC(CC)Cc1ccsc1-c1ccc(-c2cc3c(s2)-c2sc(-c4cc5c(-c6cc(Cl)c(CC(CC)CCCC	 CCCCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(cc(F)c(F)c4F)C3=C(C#N)C#N)s2)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCCC)c(-	14.96337

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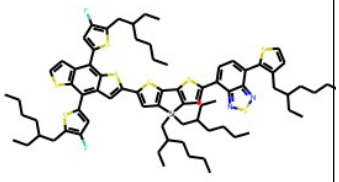
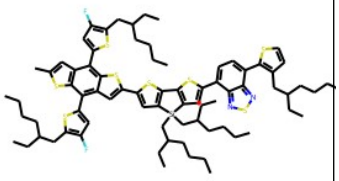
15	 CCCCC(CC)Cc1ccsc1-c1ccc(-c2cc3c(s2)-c2sc(-c4cc5c(-c6cc(F)c(CC(CC)CCCC)s6)c6sccc6c(-c6cc(F)c(CC(CC)CCCC)s6)c5s4)cc2[Si]3(CC(CC)CCCC)CC(CC)CCCC)c2nsnc12	c7ccc(C=C8C(=O)c9c(ccc(Br)c9C)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	14.96337
16	 CCCCC(CC)Cc1ccsc1-c1ccc(-c2cc3c(s2)-c2sc(-c4cc5c(-		14.94346

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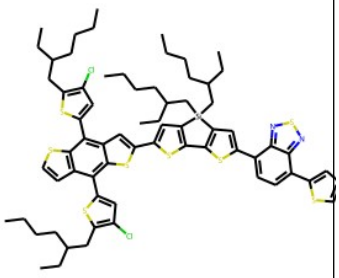
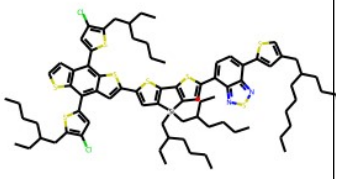
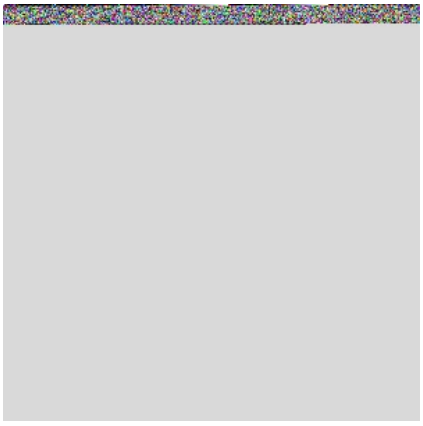
17	 CCCCC(CC)Cc1sc(-c2c3cc(-c4cc5c(s4)-c4sc(-c6ccc(-c7cccs7)c7nsnc67)cc4[Si]5(CC(CC)CCCC)CC(CC)CCCC)sc3c(-c3cc(Cl)c(CC(CC)CCCC)s3)c3ccsc23)cc1Cl		14.92056
18	 CCCCCCC(CCCC)Cc1csc(-c2ccc(-c3cc4c(s3)-c3sc(-c5cc6c(-	 CCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(cc(F)c(F)c4F)C3=C(C#N)C#N)s2)sc2c1s	14.91946

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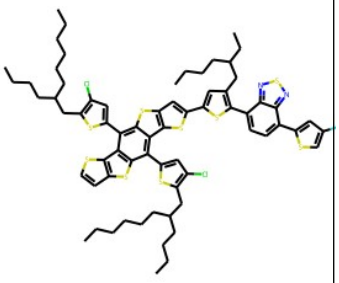
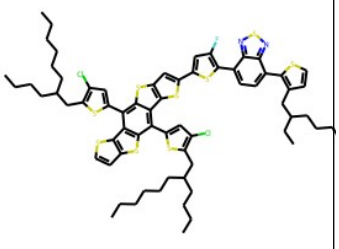
19	 CCCCCCC(CCCC)Cc1sc(-c2c3sc4cc(-c5cc(CC(CC)CCCC)c(-c6ccc(-c7cc(F)cs7)c7nsnc67)s5)sc4c3c(-c3cc(Cl)c(CC(CCCC)CCCCCC)s3)c3sc4ccsc4c23)cc1Cl		14.90425
20	 CCCCCCC(CCCC)Cc1sc(-c2c3sc4cc(-c5cc(F)c(-		14.90425

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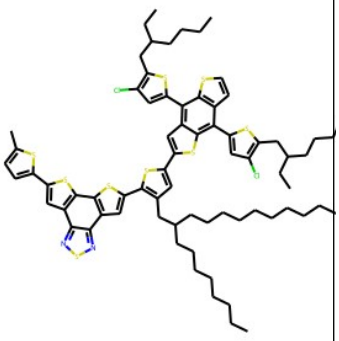
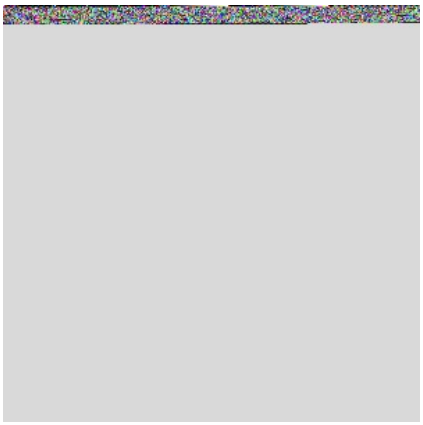
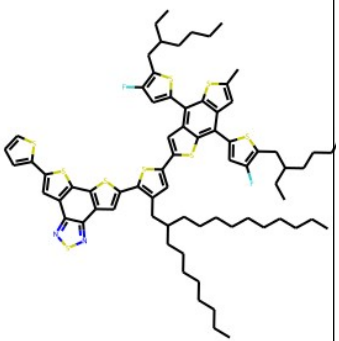
21	 CCCCCCCCCCCC(CCCCCCCC)Cc1cc(-c2cc3c(-c4cc(Cl)c(CC(CC)CCCC)s4)c4sccc4c(-c4cc(Cl)c(CC(CC)CCCC)s4)c3s2)sc1-c1cc2c3nsnc3c3cc(-c4ccc(C)s4)sc3c2s1	 CCCCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(Br)c(C)cc4C3=C(C#N)C#N)[se]2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(cc(F)c(F)c9F)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CC)CCCC)c4c3n(CC(CC)CCCC)c21	14.88351
22	 CCCCCCCCCCCC(CCCCCCCC)Cc1cc(-c2cc3c(-c4cc(F)c(CC(CC)CCCC)		14.88351

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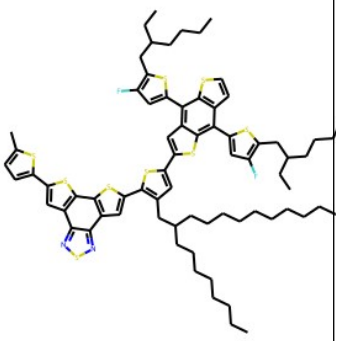
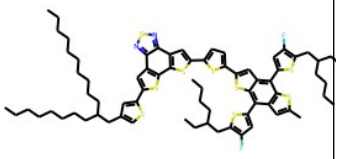
23	 CCCCCCCCCCCC(CCCCCCCC)Cc1cc(-c2cc3c(-c4cc(F)c(CC(CC)CCCC)s4)c4sccc4c(-c4cc(F)c(CC(CC)CCCC)s4)c3s2)sc1-c1cc2c3nsnc3c3cc(-c4ccc(C)s4)sc3c2s1		14.88351
24	 CCCCCCCCCCCC(CCCCCCCC)Cc1csc(-c2cc3c4nsnc4c4cc(-c5ccc(-c6cc7c(-		14.88351

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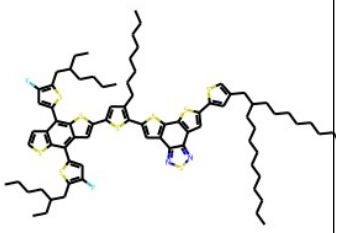
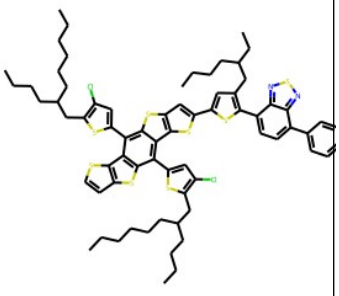
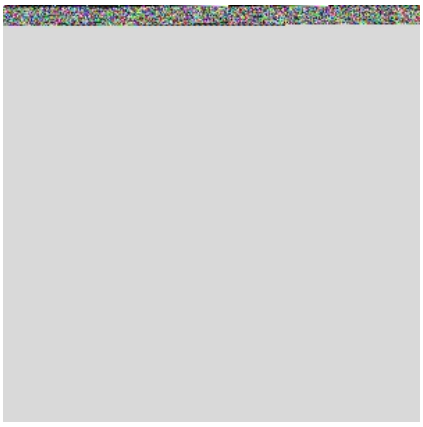
25	 CCCCCCCCCCCC(CCCCCCCCC)Cc1csc(-c2cc3c4nsnc4c4cc(-c5sc(-c6cc7c(-c8cc(F)c(CC(CC)CCCC)s8)c8sccc8c(-c8cc(F)c(CC(CC)CCCC)s8)c7s6)cc5CCCCCCCC)sc4c3s2)c1		14.86582
26	 CCCCCCC(CCCC)Cc1sc(-c2c3sc4cc(-c5cc(CC(CC)CCCC)c(-c6ccc(-	 CCCCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(cc(F)c(F)c4F)C3=C(C#N)C#N)s2)sc2c1sc1c3c4nccnc4c4c5sc6c(CCCCCCCCCCC)c(-	14.85526

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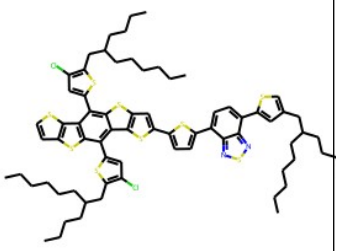
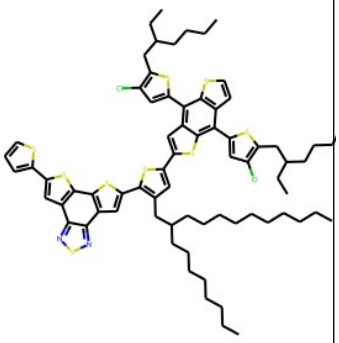
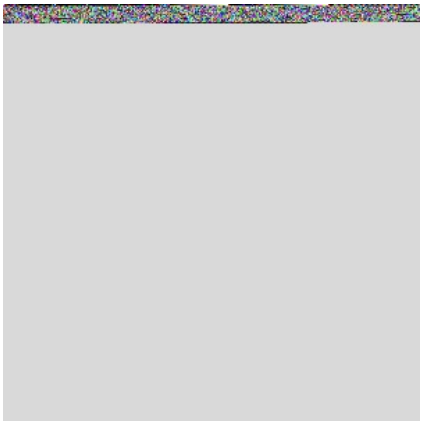
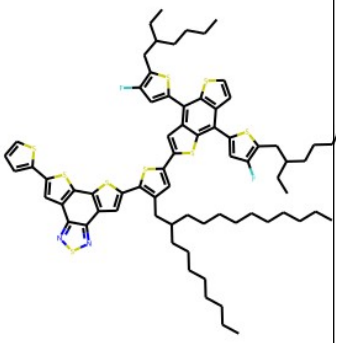
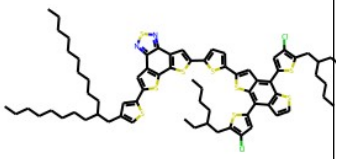
27	 CCCCCCC(CCCC)Cc1csc(-c2ccc(-c3ccc(-c4cc5sc6c(-c7cc(Cl)c(CC(CCCC)CCCCCC)s7)c7c(sc8ccsc87)c(-c7cc(Cl)c(CC(CCCC)CCCCCC)s7)c6c5s4)s3)c3nsnc23)c1	 CCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4c(cc(F)c(F)c4F)C3=C(C#N)C#N)s2)sc2c1sc1c3c4nsnc4c4c5sc6c(CCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(ccc(Br)c9C)C8=C(C#N)C#N)[se]7)[se]c6c5n(CC(CCCC)CCCCCC)c4c3n(CC(CCCC)CCCCCC)c21	14.84969
28	 CCCCCCCCCCC(CCCCCCCC)Cc1cc(-c2cc3c(-c4cc(Cl)c(CC(CC)CCCC	 CCCCCCCCCCCc1c(-c2ccc(C=C3C(=O)c4cc(Br)c(C)cc4C3=C(C#N)C#N)[se]2)sc2c1	14.83968

	)s4)c4sccc4c(-c4cc(Cl)c(CC(CC)CCCC)s4)c3s2)sc1-c1cc2c3nsnc3c3cc(-c4cccs4)sc3c2s1		
29	 CCCCCCCCCCCC(CCCCCCCC)Cc1cc(-c2cc3c(-c4cc(F)c(CC(CC)CCCC)s4)c4sccc4c(-c4cc(F)c(CC(CC)CCCC)s4)c3s2)sc1-c1cc2c3nsnc3c3cc(-c4cccs4)sc3c2s1	sc1c3c4nsnc4c4c5sc6c(CCCCCCCCCCCC)c(-c7ccc(C=C8C(=O)c9c(cc(F)c(F)c9F)C8=C(C#N)C#N)[se]7)sc6c5n(CC(CC)CCCC)c4c3n(CC(CC)CCCC)c21	14.83968
30	 CCCCCCCCCCCC(CCCCCCCC)Cc1csc(-c2cc3c4nsnc4c4cc(-c5ccc(-c6cc7c(-		14.83968

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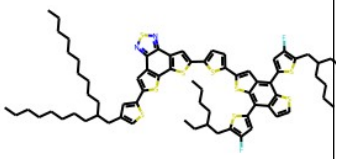
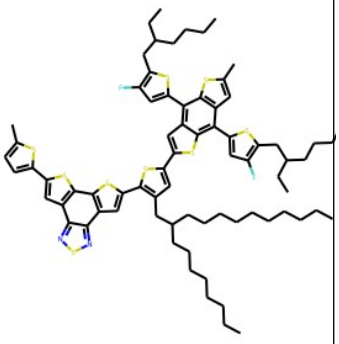
31	 CCCCCCCCCCCC(CCCCCCCC)Cc1csc(-c2cc3c4nsnc4c4cc(-c5ccc(-c6cc7c(-c8cc(F)c(CC(CC)CCCC)s8)c8sccc8c(-c8cc(F)c(CC(CC)CCCC)s8)c7s6)s5)sc4c3s2)c1		14.83968
32	 CCCCCCCCCCCC(CCCCCCCC)Cc1cc(-c2cc3c(-c4cc(F)c(CC(CC)CCCC)s4)c4sc(C)cc4c(-c4cc(F)c(CC(CC)CCCC)		14.79273

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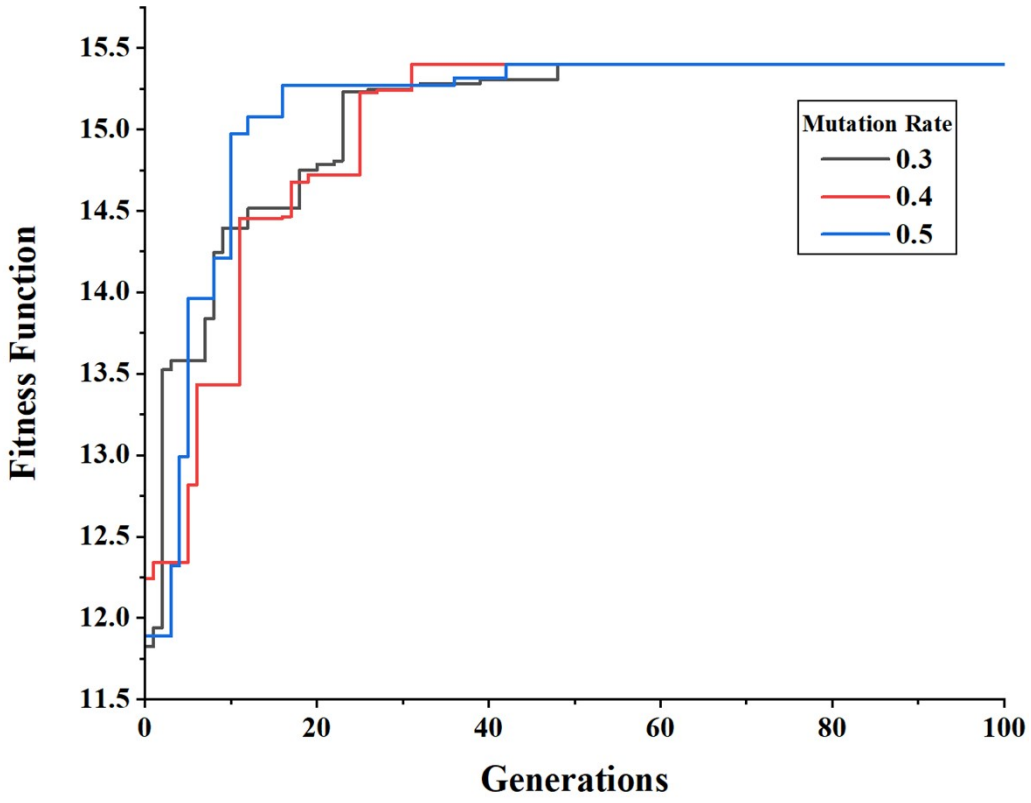


Figure S1 GA iteration process of the A_1-π_1-D-π_2-A_2 type acceptor molecules under different mutation probabilities.

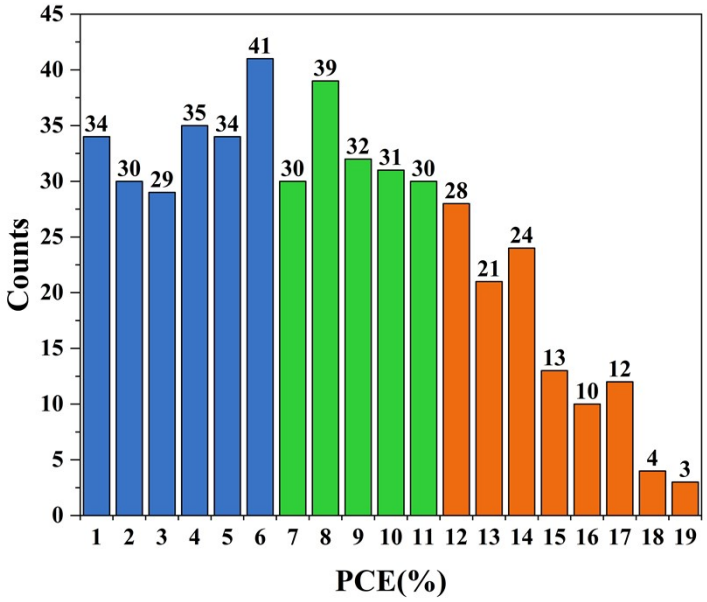
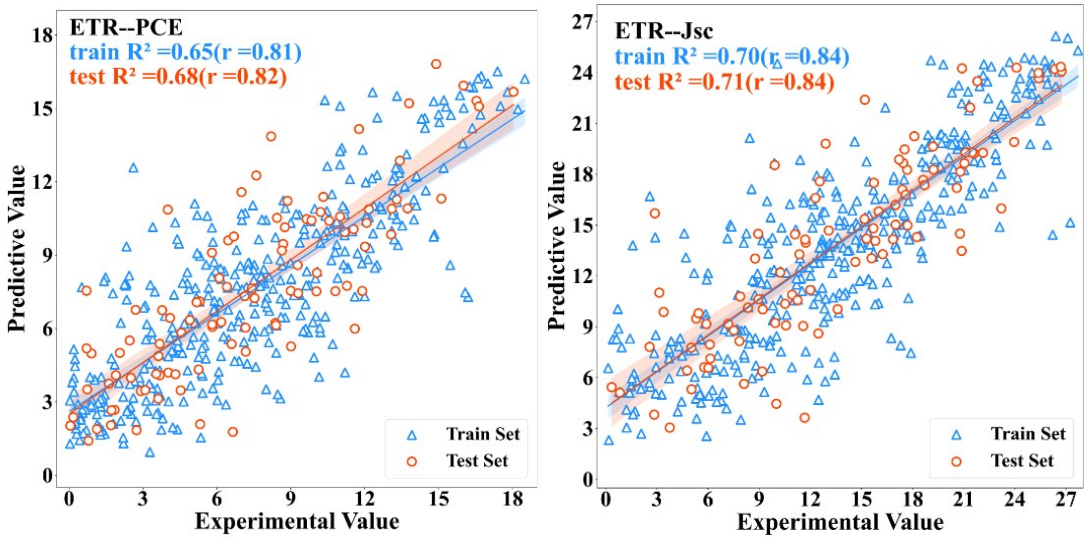


Figure S2 Experimental PCE distribution of NFA OSCs in the dataset.



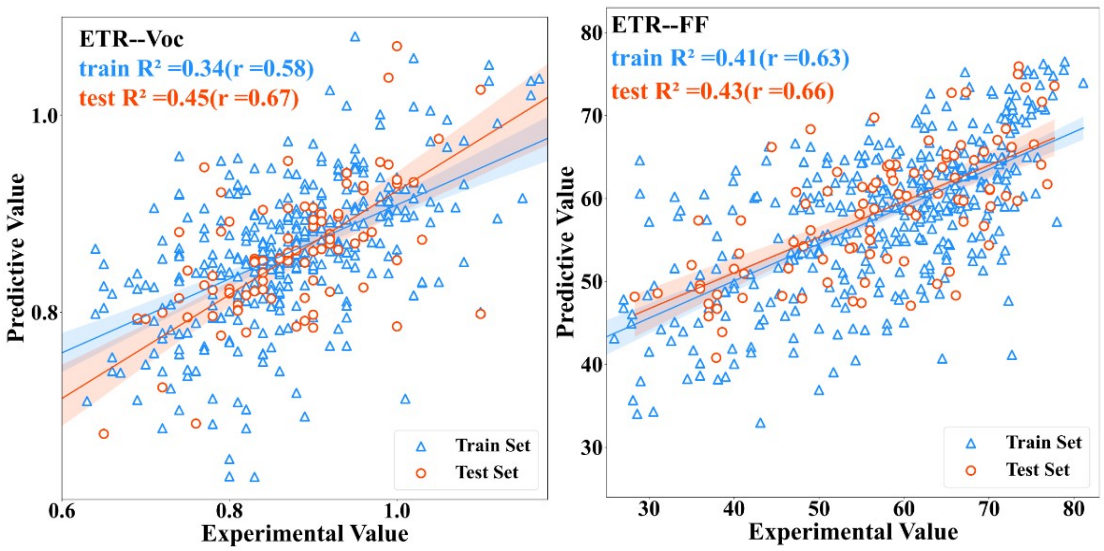


Figure S3: The RF and ETR algorithms were used to predict the photovoltaic performance parameters (PCE, V_{OC}, J_{SC}, and FF) of OSCs on the training set (with 384 data points) and the test set (with 96 data points). The blue color represents the prediction results on the training set, while the red color represents those on the test set. The corresponding R^2 and r are given in the upper left corner. The blue and red areas indicate the error ranges of the corresponding fitting lines.

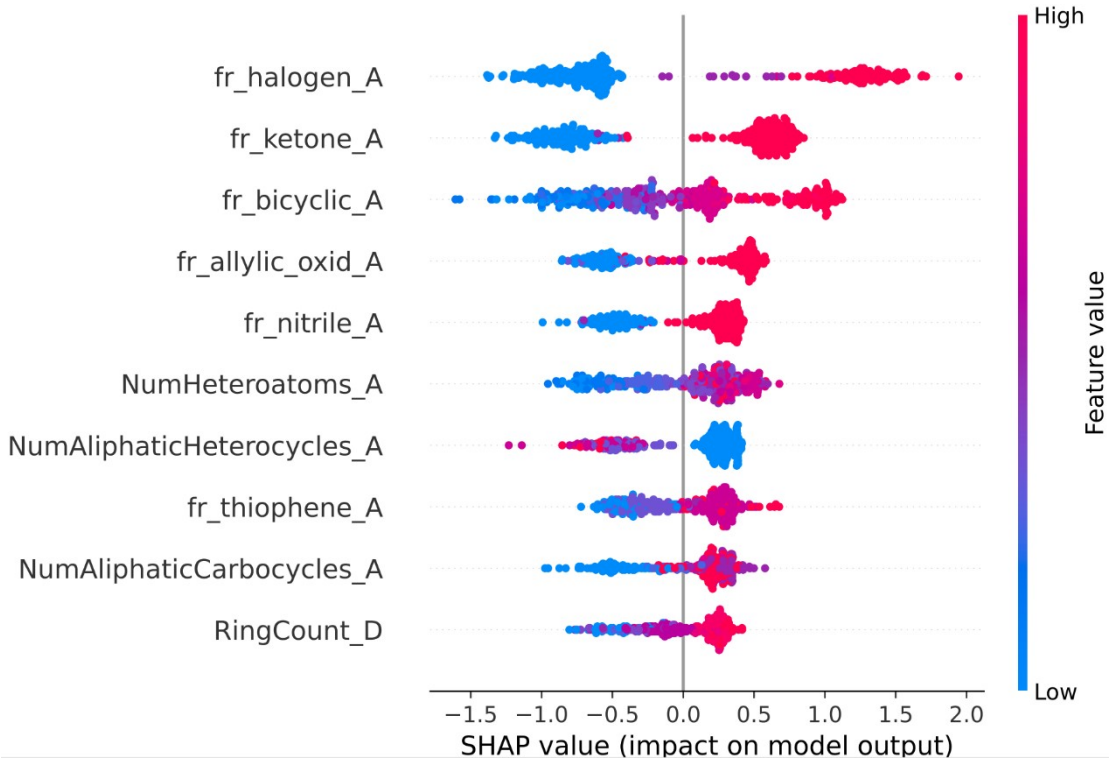


Figure S4 The SHAP importance ranking of 43 molecular structure descriptors for J_{SC} (mA/cm²) in the RF algorithm.

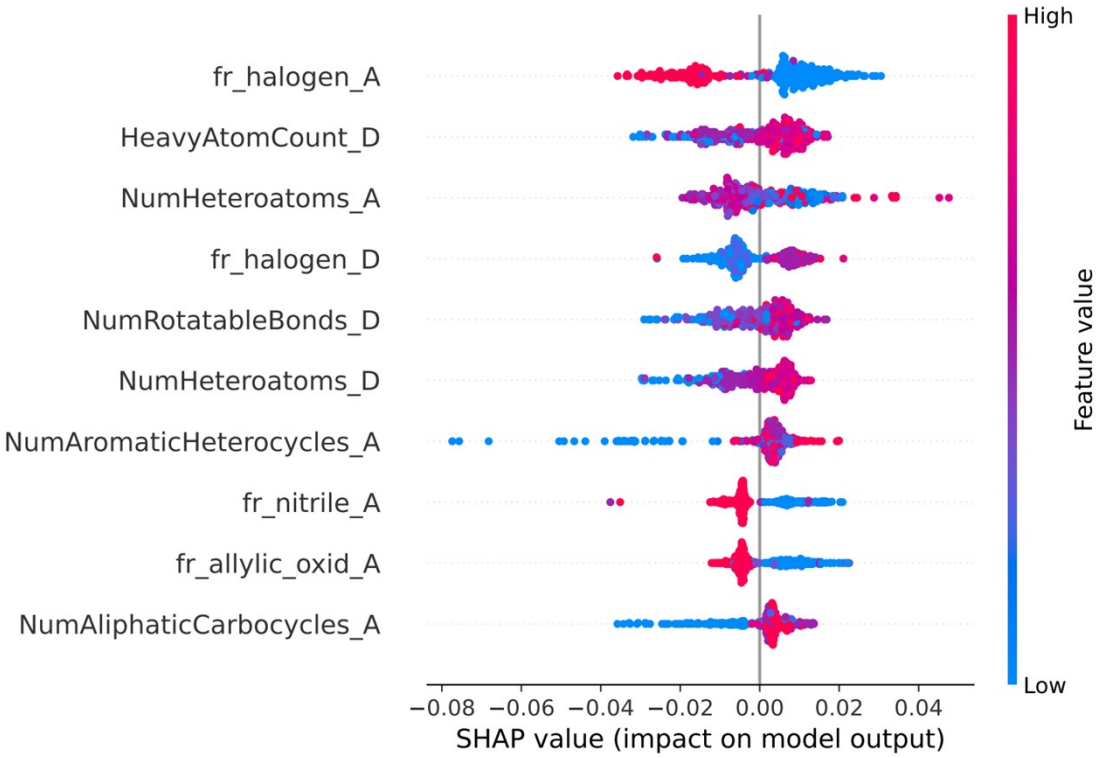


Figure S5: The SHAP importance ranking of 43 molecular structure descriptors for V_{OC} (V) in the RF algorithm.

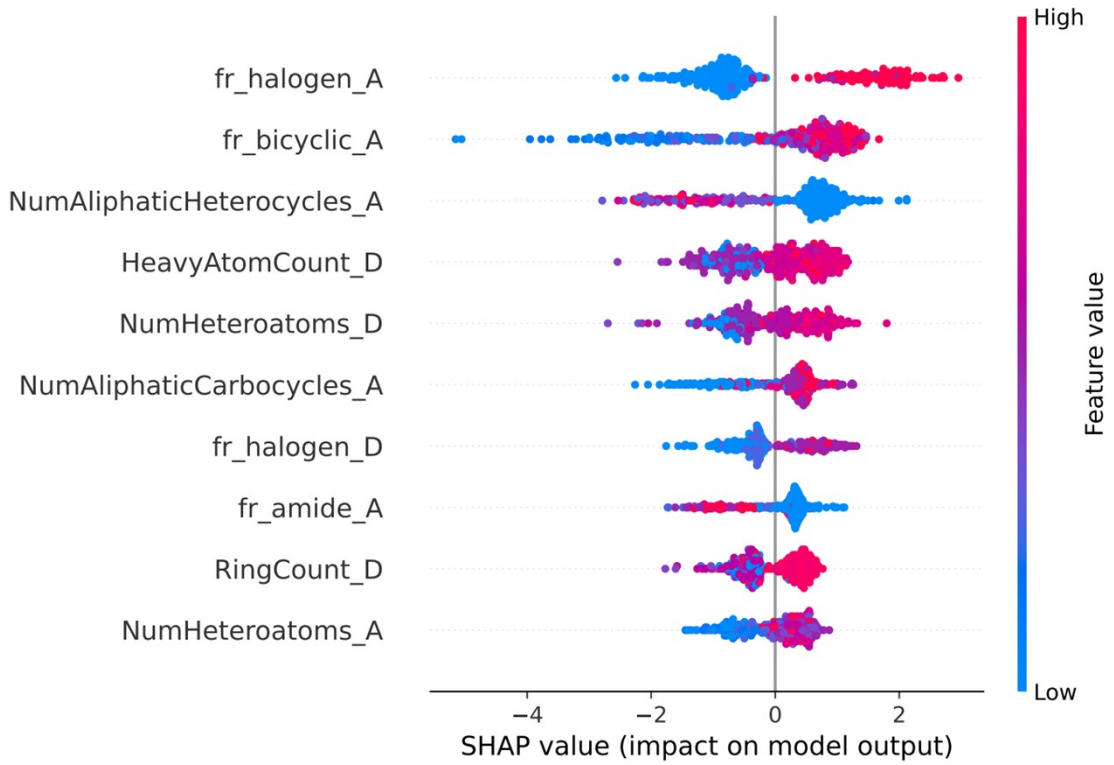


Figure S6: The SHAP importance ranking of 43 molecular structure descriptors for FF (%) in the RF algorithm.

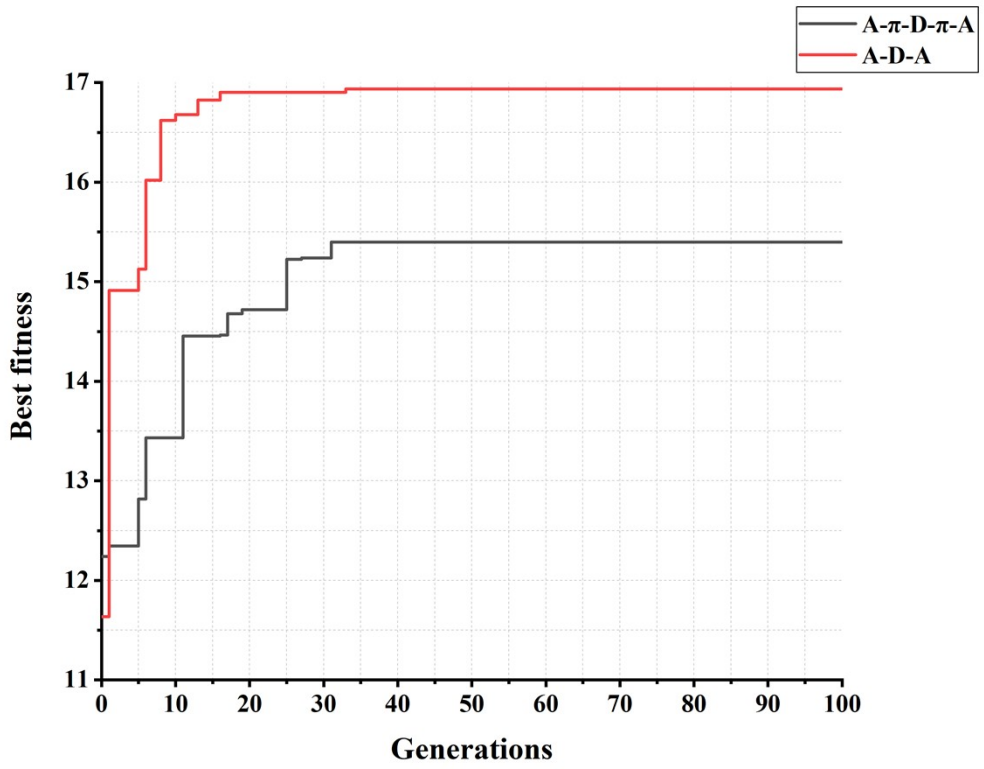


Figure S7 GA iteration process of acceptor molecules with the A_1-π_1-D-π_2-A_2 and A_1-D-A_2 types.

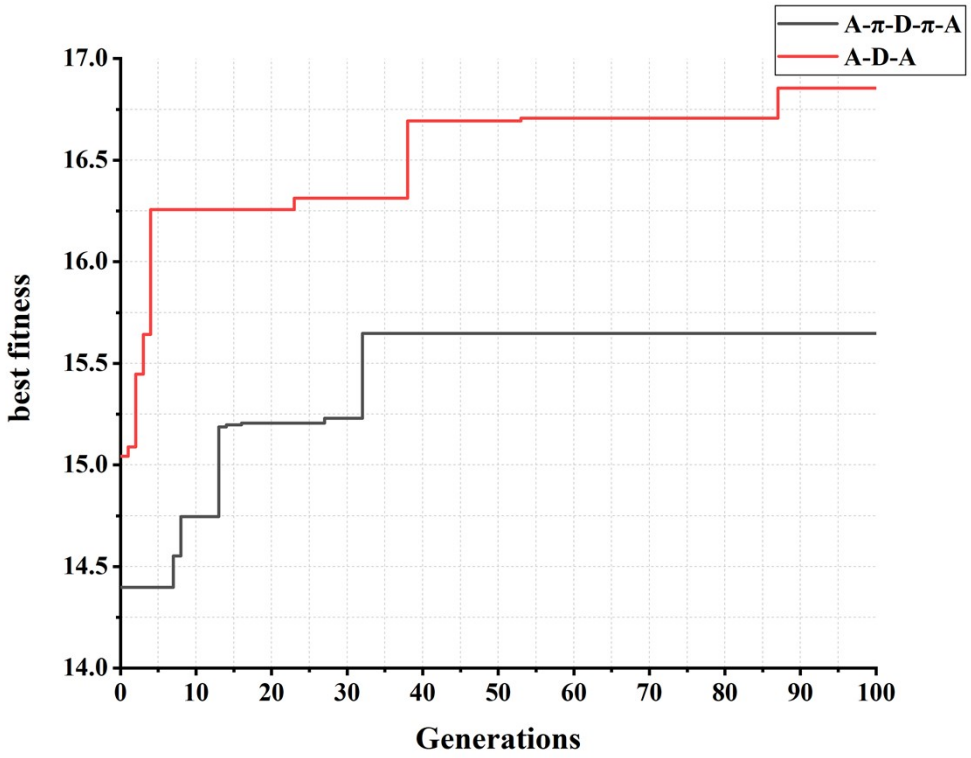


Figure S8 GA iteration process of the D-π_1-A-π_2 type donor molecules paired with acceptor molecules of the A_1-π_1-D-π_2-A_2 and A_1-D-A_2 types.