Electronic Supplementary Information

Development of a quantum chemical descriptor expressing aromatic/quinoidal character for designing narrow-bandgap π-conjugated polymers

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A. Determining the degree of oligoacetylene polymerization

To determine the degree of oligoacetylene polymerization in eq. 2, we calculated the reaction energy in eq. 2 for n = 1–11. The reaction energy converged to 31.4 kcal mol^{-1} at n = 8, as shown in Figure S1. Therefore, the degree of polymerization was determined to be n = 8.

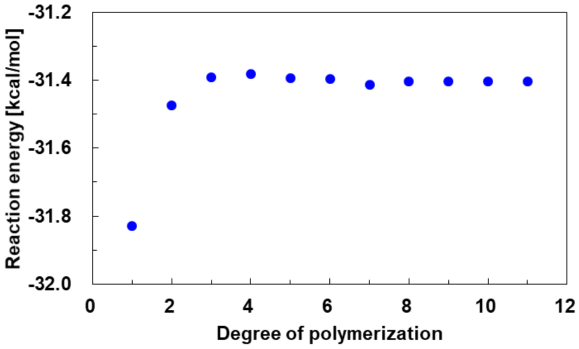


Figure S1. Dependence of reaction energy in the hydrogenation of oligoacetylene on the degree of polymerization.

B. Benchmark calculation of QSE and bandgap

We evaluated the QSE for 10 typical monomers by the single-point calculation at the CCSD(T)/6-311G(d,p) level, using the structure optimized at the ωB97X-D/6-311G(d,p) level. The trend of QSE with ωB97X-D was found to be in good agreement with that with CCSD(T), although the former includes a systematic error of about 3 kcal mol^{-1} compared to the latter, as shown in Figure S2.

In addition, the ωB97X-D can be considered a reliable method to calculate the QSE for the following reasons. (1) The computational cost to calculate the QSE of 268 monomers at the CCSD(T) level is too high, so DFT methods such as ωB97X-D are more suitable. (2) The long-range correction and empirical dispersion correction can be improved to more accurately calculate various properties, such as the reaction energy, that are problematic for conventional functionals such as B3LYP.[1–7] The ωB97X-D includes both the long-range correction and empirical dispersion correction. (3) Various benchmark studies showed that, in the benchmark set of homodesmotic reactions (PlatonicHD6), the reaction energy obtained by ωB97X-D is in good agreement with the reference energy obtained by W1-F12.[8]

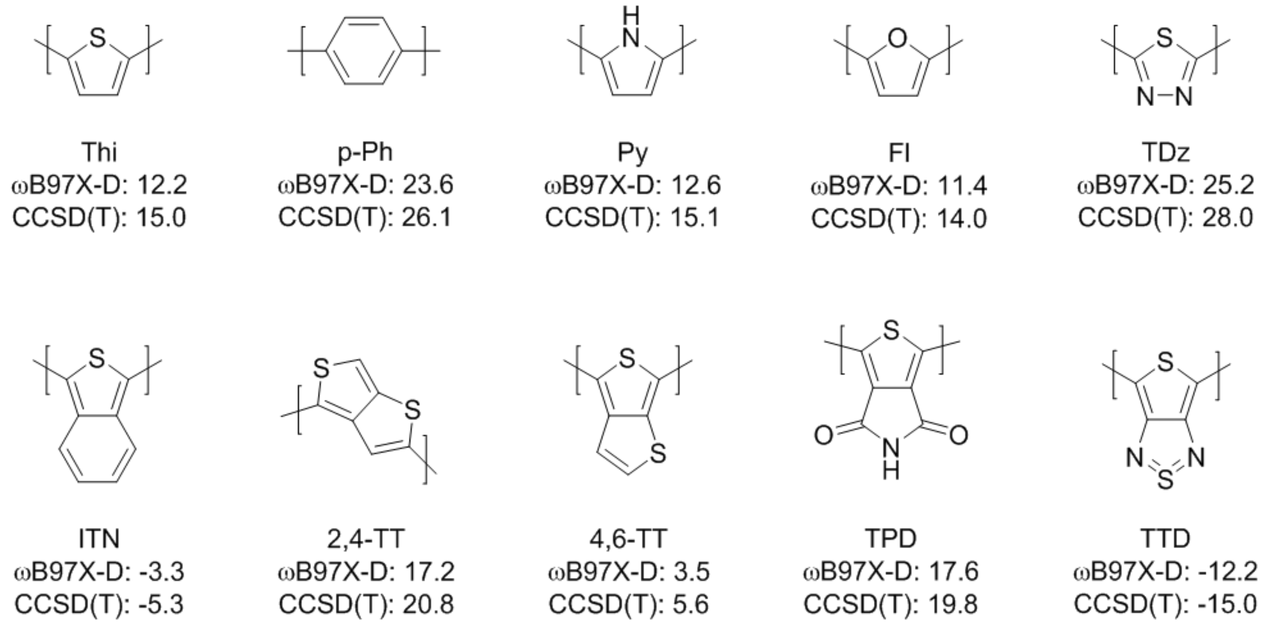


Figure S2. QSE values calculated by the ωB97X-D/6-311G(d,p) and CCSD(T)/6-311G(d,p) functionals for 10 typical monomers.

We carried out benchmark calculation for the bandgap of the 268 homopolymers using the CAM-B3LYP,[9] HSE06,[10] and M11-L[11] functionals. The plots of bandgap against QSE are shown in Figure S3. The three functionals have the same trend as that of B3LYP, that is, the bandgap is the lowest when QSE = 0. This means that the choice of functional does not influence our main conclusion, that narrow-bandgap polymers can be designed with QSE = 0. On the other hand, the calculated bandgap in CAM-B3LYP (2.7–7.3 eV) was larger than those in B3LYP (0.7–4.8 eV), HSE06 (0.3–4.4 eV), and M11-L (0.0–3.7 eV). The issue of the spreading bandgap in LC-DFT such as CAM-B3LYP has been pointed out by several studies.[12,13] In addition, the bandgap calculated with these three functionals for poly(thiophene), poly(pyrrole), and poly(furan) are summarized in Table S1. Among them, B3LYP showed the best agreement with the experimental optical bandgap. It is also known that bandgap calculated with the B3LYP functional with one-dimensional PBC has good agreement with the experimental optical bandgap.[14,15] Therefore, B3LYP was chosen for the bandgap calculations in this work. Again, we emphasize that the main conclusion (that the bandgap is the lowest when QSE = 0) is not influenced by the choice of functionals.

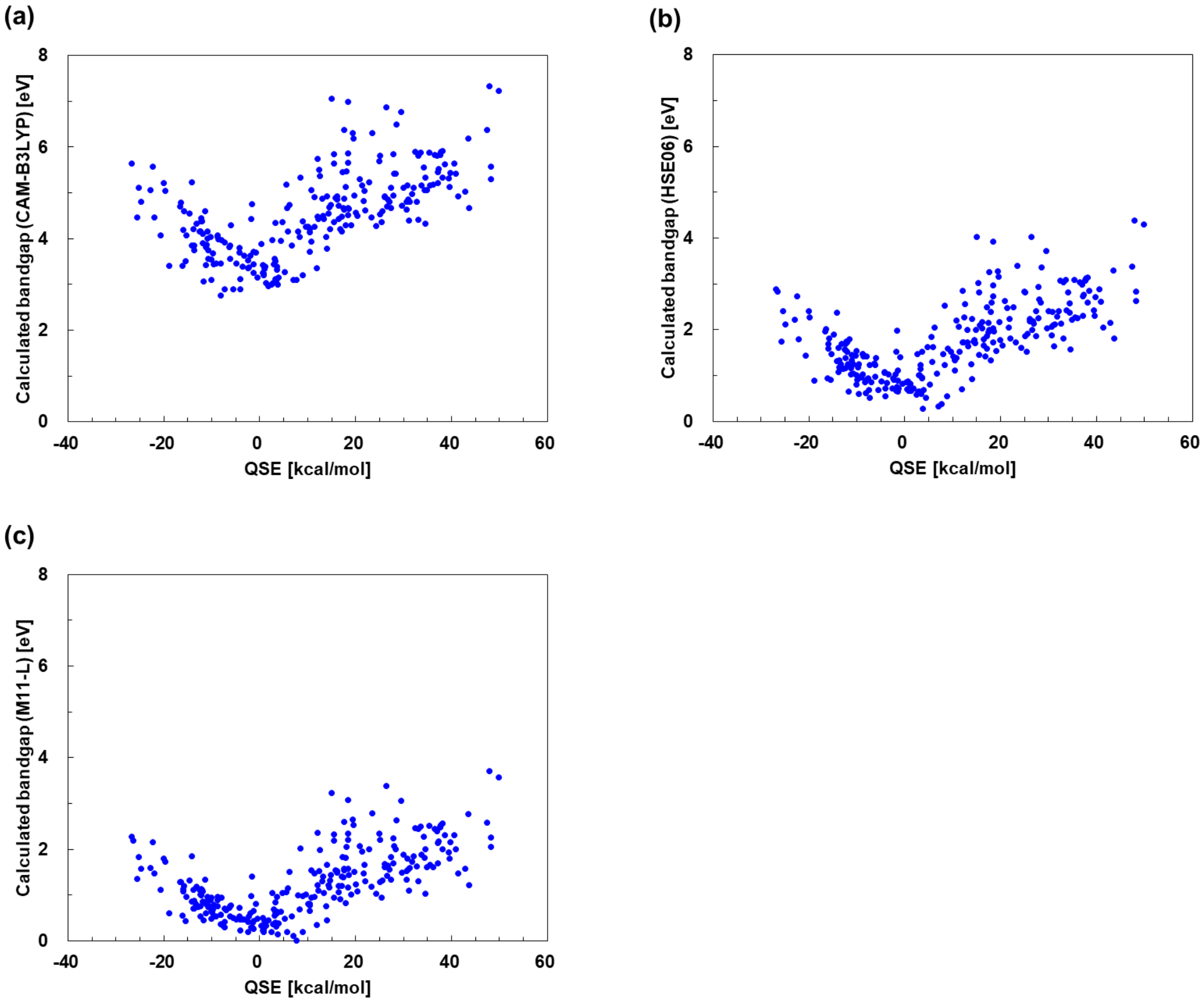


Figure S3. Correlation between the QSE and bandgap in homopolymers. The bandgap was calculated by (a) CAM-B3LYP, (b) HSE06, and (c) M11-L combined with the 6-31G(d,p) basis set.

Table S1. Bandgaps for typical conjugated polymers (eV).

Polymer	B3LYP	CAM-B3LYP	HSE06	M11-L	Exp. optical bandgap
Poly(thiophene)	2.05	4.45	1.70	1.21	2.1[16]
Poly(pyrrole)	2.90	5.37	2.52	1.96	2.8[14]
Poly(furan)	2.41	4.90	2.05	1.46	2.35[17]

C. Recipe of QSE calculation

Below is a description of the calculation procedure of QSE.

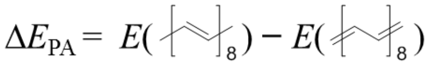
(1) Structural optimization and vibrational analysis are carried out with ωB97X-D/6-311G(d,p) for the dimethylated and dimethyleneated monomers, in which the two linkages of the monomer unit are substituted with methyl or methylene groups, respectively. The route section of Gaussian 09 or Gaussian 16 is as follows:

```
# opt freq uwb97xd/6-311G(d,p) int=ultrafine guess=mix
```

where unrestricted wavefunction and guess=mix option are used because a few monomers are singlet diradicals in the ground state. The int=ultrafine option is used because the default setting of integral grid is relatively coarse in Gaussian 09. In Gaussian 16, this option is not necessary because it is the default setting.

(2) The energy difference Δ*E* between the methyl and methylene disubstituted monomers is calculated by adding the zero-point correction.

(3) QSE is calculated by QSE = $\Delta E - 763.06$ (kcal mol^{-1}). The value –763.06 kcal mol^{-1} is the energy difference ΔE_{PA} between methyl and methylene disubstitution of the polyacetylene oligomer (n = 8) (eq 6) obtained by ωB97X-D/6-311G(d,p), after adding the zero-point correction. It is necessary to recalculate ΔE_{PA} when one wants to use calculation methods such as B3LYP.



(S1)

D. LASSO regression

In this work, the least absolute shrinkage and selection operator (LASSO)[18] as a linear regression method was performed for data mining to find monomer features that influence the QSE. Variables that are determined to be less informative are eventually omitted from the regression equation in LASSO. Thus, it is an efficient technique for feature selection. The LASSO was defined as:

$$\widehat{\beta_{LASSO}} = \underset{\beta}{\operatorname{argmin}} \left\{ \frac{1}{2}\sum_{n=1}^{N}\left(y_i - \beta_0 + \sum_{j=1}^{p} x_{ij}\beta_{ij} \right)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right\} \quad (\mathrm{S2}),$$

where x and y are the explanatory and objective variables, respectively, β_0 is the intercept, β is the regression coefficient. λ is the complexity parameter, which is determined at the maximum value satisfying minimization of the root mean square error (RMSE) and maximization of R^2 of the linear regression. The data were verified by 10-folds cross-validation. LASSO regression was performed by the Orange software[19] for data mining and machine learning.

E. C–C bond lengths of poly(thienoisoindigo)

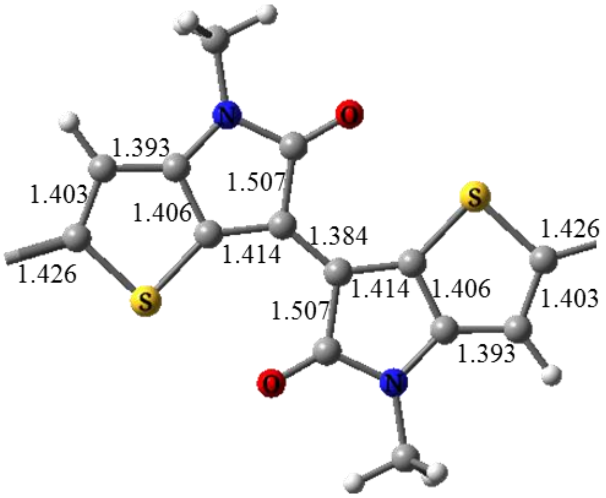


Figure S4. Calculated C–C bond lengths in Å of poly(thienoisoindigo).

F. Investigation of size effect and size correction for QSE

In order to confirm the monomer unit size dependence of QSE, the QSE values were obtained from monomers and their dimers, and compared with each other in Figure S5. Although the two sets of QSEs are linearly correlated, the dimers have larger absolute QSE values than the monomers. From this result, it became clear that QSE has a monomer size dependence.

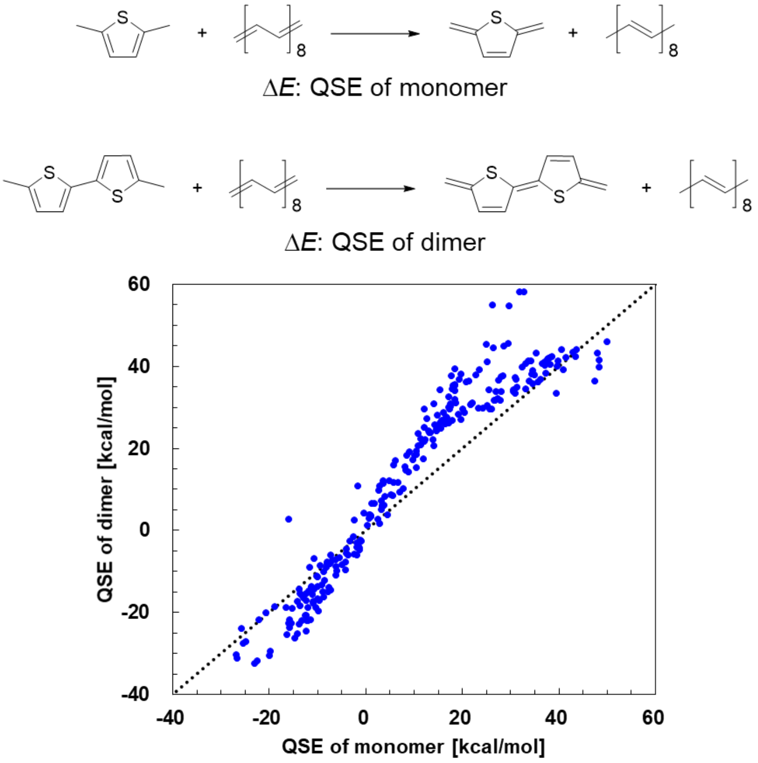


Figure S5. Comparison of QSE of monomers and dimers.

We attempted to correct the monomer unit size dependence of QSE using the π-electron number. The size-corrected QSE ($\mathrm{QSE_{SC}}$) was defined by eq S3.

$$\mathrm{QSE_{SC}} = \mathrm{QSE} / A \qquad \text{(S3)}$$

where A is a function of the π-electron number, which is defined using four different patterns: (a) the π-electron number of the shortest path between the linking sites of the monomer unit, (b) the total number of π-electrons of the monomer unit, (c) the square root of (a), and (d) the square root of (b).

Removing the monomer unit size dependence of QSE means that the values of QSE$_{SC}$ obtained from the monomer and its dimer should be equal. Therefore, the QSE$_{SC}$ values calculated using the four patterns of *A* were compared for the monomers and dimers (Figure S6). The QSE and QSE$_{SC}$ show better linear correlation for patterns (c) and (d) with a slope close to 1. However, in (d) there remains an ambiguity in the definition of π-electron number (e.g. whether or not to include the lone electron pair on the EDOT ether oxygen. In (d), the lone electron pair on the EDOT ether oxygen was not included). Therefore, we decided to use (c) for *A*.

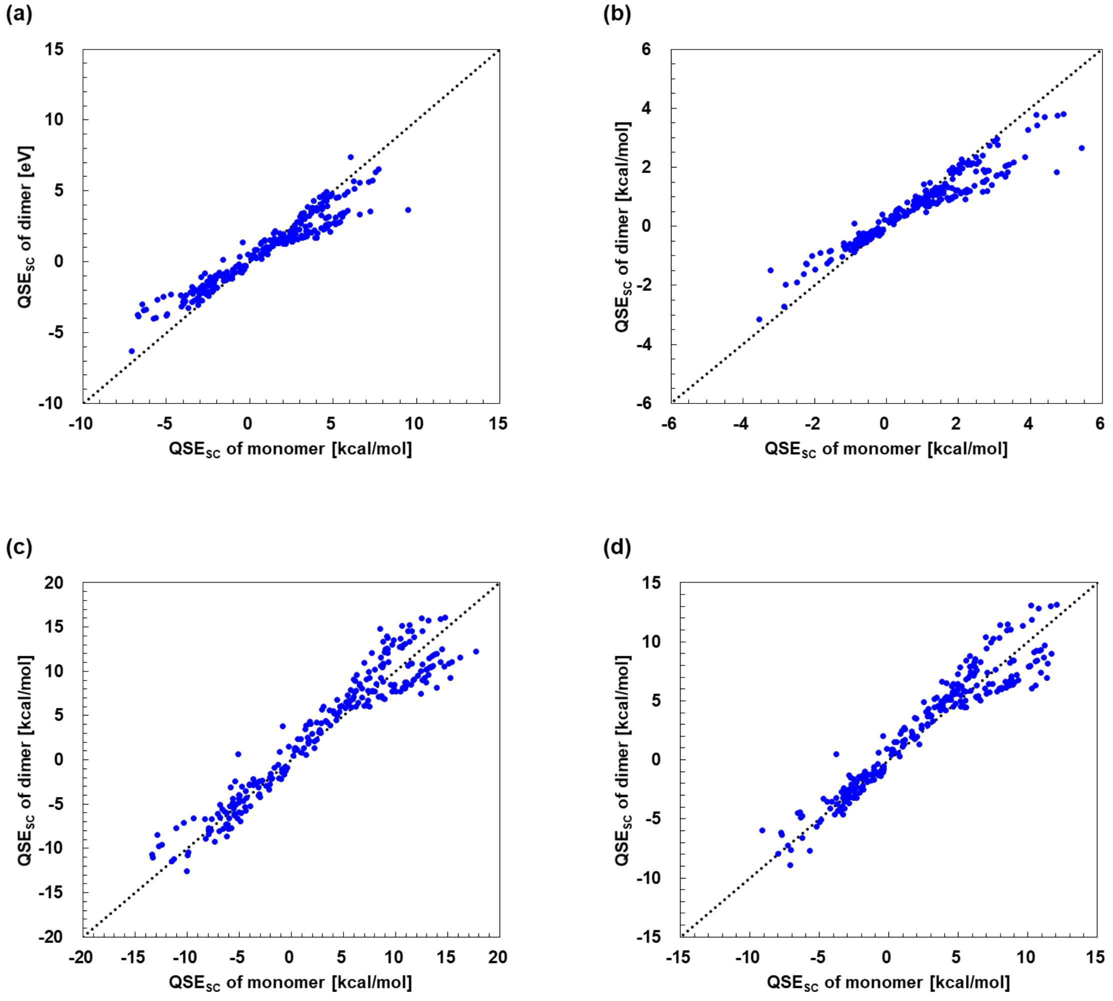


Figure S6. Comparison of size-corrected QSE (QSE$_{SC}$) values of monomer and dimer using four patterns for *A*.

Note that in homopolymers, the QSE of dimers is a good way to include the effect of torsion angle between the monomer units. However, in alternating copolymers, the amount of calculation needed to obtain the QSE of dimers is enormous, because 4950 copolymers can be created from the combination of 100 kinds of monomers. For this reason, we consider that the QSE of dimers is not suitable for the bandgap prediction of copolymers.

The theoretical bandgaps of various homopolymers are plotted against $\mathrm{QSE_{SC}}$ in Figure S7. Compared with QSE, the correlation between $\mathrm{QSE_{SC}}$ and the theoretical bandgap was improved, especially in the region where the QSE is positive and large. Although the reason for this functional form of *A* is unknown and there is room for improvement, adding the size correction is important for improving the bandgap prediction ability of QSE. In addition, we confirmed that using $\mathrm{QSE_{SC}}$ does not influence the conclusions for the relationship between QSE and monomer structures, as shown in Figure S8.

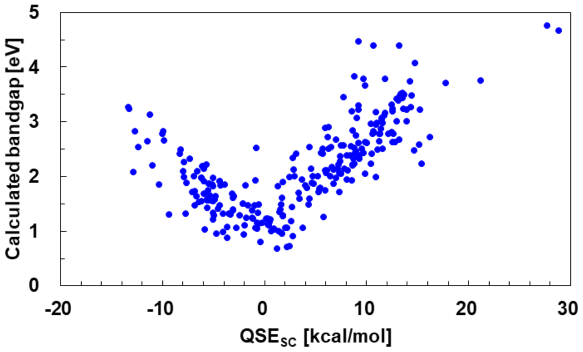


Figure S7. Correlation between the size-corrected QSE ($\mathrm{QSE_{SC}}$) and bandgap in 268 homopolymers.

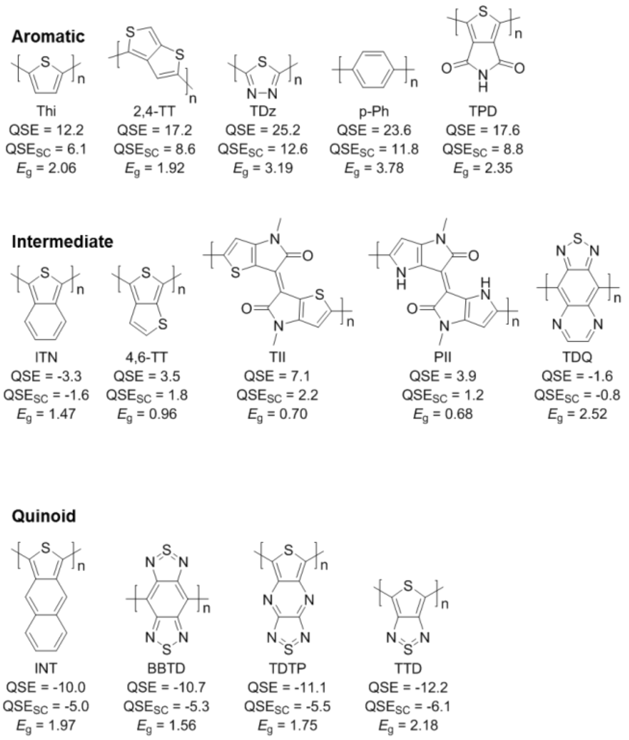


Figure S8. Chemical structure, QSE in kcal mol^{-1}, QSE$_{\mathrm{SC}}$ in kcal mol^{-1}, and the calculated bandgap (E_{g}) in eV of a few examples of aromatic (having larger positive QSE), quinoidal (having larger negative QSE), and their intermediate monomer units.

We tried to apply QSE$_{\mathrm{SC}}$ to alternating copolymers and periodic copolymers with various monomer ratios. The QSE$_{\mathrm{SC}}$ of the copolymers (QSE$_{\mathrm{SC,CO}}$) is expressed by equations S4 and S5.

$$\mathrm{QSE_{SC,CO}} = (\mathrm{QSE_{SC,1}} + \mathrm{QSE_{SC,2}}) / 2 \qquad \text{(S4)}$$

$$\mathrm{QSE_{SC,CO}} = \mathrm{QSE_{SC,1}} \cdot w_1 + \mathrm{QSE_{SC,2}} \cdot w_2 \qquad \text{(S5)}$$

where S4 is the special case of alternating copolymers, and S5 is the case of periodic copolymers with various monomer ratios. QSE$_{\mathrm{SC,1}}$ and QSE$_{\mathrm{SC,2}}$ are the QSE$_{\mathrm{SC}}$ values of monomer 1 and 2, respectively, and w_1 and w_2 are the respective mole fractions. The plot of bandgap against QSE$_{\mathrm{SC}}$ of alternate copolymers is shown in Figure S9. A few examples of alternating copolymers with narrow calculated bandgaps are shown in Figure S10. The correlation between QSE$_{\mathrm{SC}}$ and the theoretical bandgap was improved from that of QSE. The plot of the bandgap against QSE$_{\mathrm{SC}}$ of periodic copolymers with various monomer ratios is shown in Figure S11, while the numerical data are summarized in Tables

S2 and S3. We confirmed that using QSE_{SC} does not influence the conclusions for the relationship between QSE and monomer structures in alternate copolymers and periodic copolymers. In addition, we also confirmed that the correlations between QSE_{SC} and HOCO-LUCO levels were similar as those of QSE, as shown in Figure S12.

Based on the above assessment of QSE and QSE_{SC}, narrow-bandgap polymers can be designed by combining monomers in such a way that the averaged QSE or QSE_{SC} becomes close to zero. In other words, the use of QSE is sufficient for the design of narrow-bandgap polymers and it is not necessary to use QSE_{SC}. The QSE_{SC} is more suitable when predicting a polymer expressing any value of bandgap.

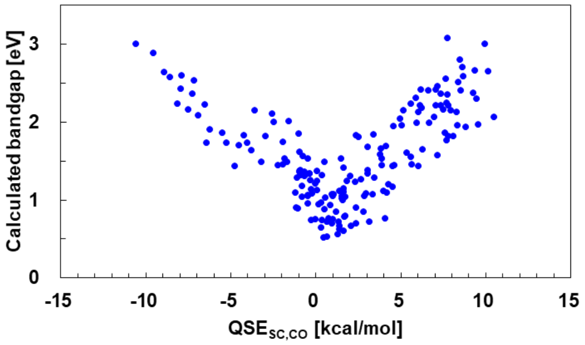
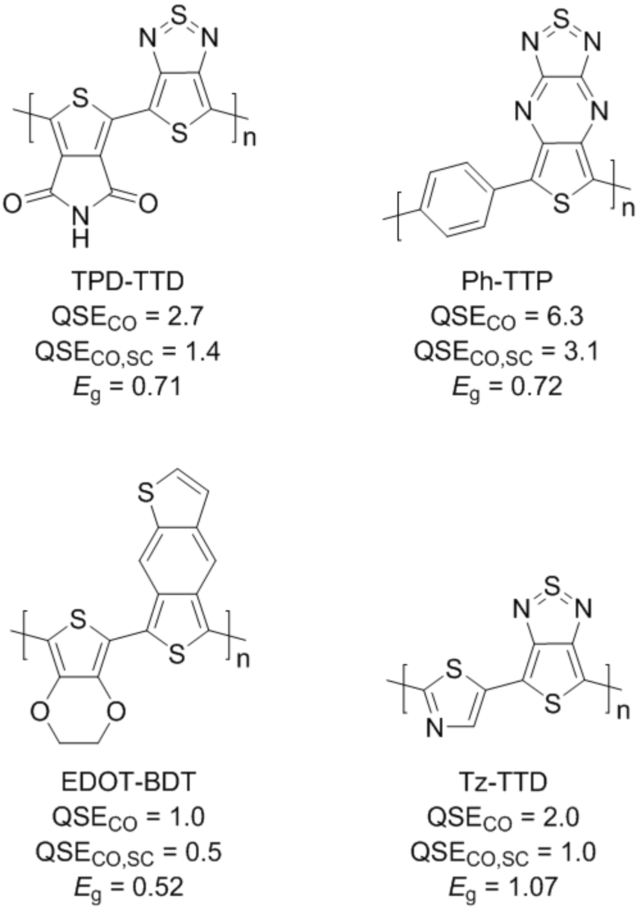


Figure S9. Correlation between the size-corrected QSE_{CO} ($QSE_{SC,CO}$) and the bandgap in 179 alternate copolymers.



TPD-TTD
$QSE_{CO} = 2.7$
$QSE_{CO,SC} = 1.4$
$E_g = 0.71$

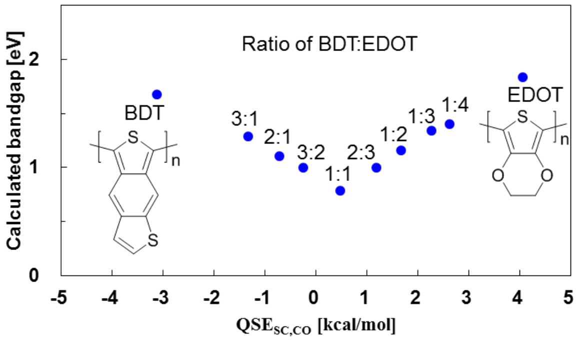
Ph-TTP
$QSE_{CO} = 6.3$
$QSE_{CO,SC} = 3.1$
$E_g = 0.72$

EDOT-BDT
$QSE_{CO} = 1.0$
$QSE_{CO,SC} = 0.5$
$E_g = 0.52$

Tz-TTD
$QSE_{CO} = 2.0$
$QSE_{CO,SC} = 1.0$
$E_g = 1.07$

Figure S10. Chemical structure, QSE_{CO} in kcal mol^{-1}, $QSE_{SC,CO}$ in kcal mol^{-1}, and the calculated bandgap (E_g) in eV for examples of narrow-bandgap alternating copolymers.

(a)



(b)

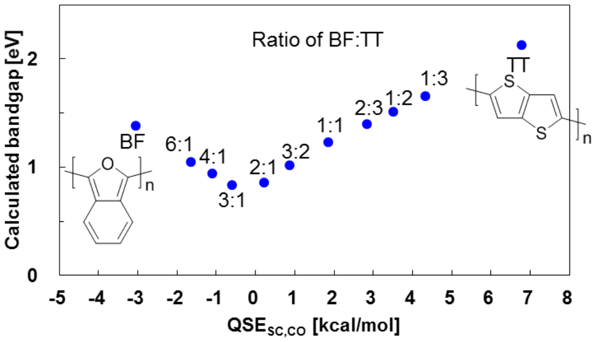


Figure S11. Calculated bandgap against QSE$_{SC,CO}$ for (a) BDT-EDOT and (b) BF-TT periodic copolymers with different ratios.

Table S2. Calculated bandgap, QSE$_{\mathrm{CO}}$, and QSE$_{\mathrm{SC,CO}}$ of the BDT-EDOT periodic copolymers.

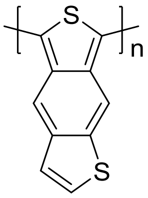
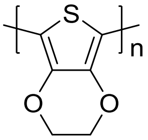
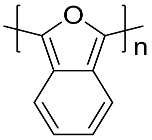
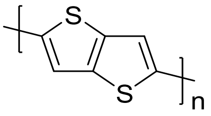
Structure	Ratio of BDT:EDOT	QSE$_{\mathrm{CO}}$ [kcal/mol]	QSE$_{\mathrm{SC,CO}}$ [kcal/mol]	Bandgap [eV]
 BDT  EDOT	1:0	-6.2	-3.1	1.68
	3:1	-2.6	-1.3	1.29
	2:1	-1.4	-0.7	1.11
	3:2	-0.5	-0.2	1.00
	1:1	0.9	0.5	0.79
	2:3	2.4	1.2	1.00
	1:2	3.3	1.7	1.16
	1:3	4.5	2.3	1.34
	1:4	5.3	2.6	1.40
	0:1	8.1	4.1	1.84

Table S3. Calculated bandgap, QSE$_{\mathrm{CO}}$, and QSE$_{\mathrm{SC,CO}}$ of the BF-TT periodic copolymers.

Structure	Ratio of BF:TT	QSE$_{\mathrm{CO}}$ [kcal/mol]	QSE$_{\mathrm{SC,CO}}$ [kcal/mol]	Bandgap [eV]
 BF  TT	1:0	-6.1	-3.1	1.38
	6:1	-2.9	-1.7	1.05
	4:1	-1.6	-1.1	0.94
	3:1	-0.4	-0.6	0.83
	2:1	1.6	0.2	0.86
	3:2	3.0	0.9	1.02
	1:1	5.2	1.9	1.23
	2:3	7.5	2.8	1.40
	1:2	9.0	3.5	1.52
	1:3	10.9	4.3	1.66
	0:1	16.6	6.8	2.13

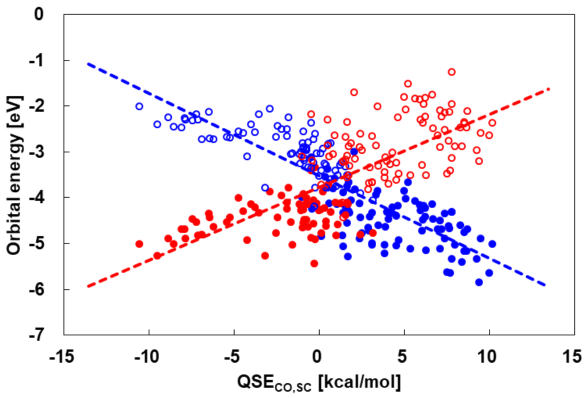
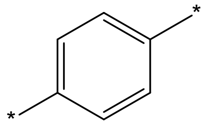
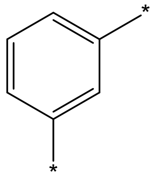
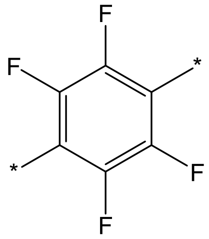
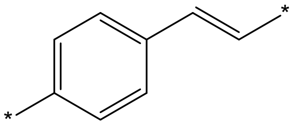
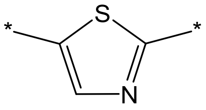
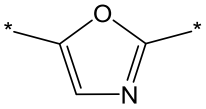
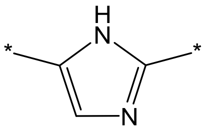
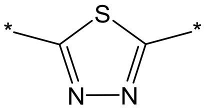
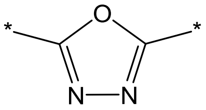
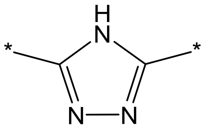
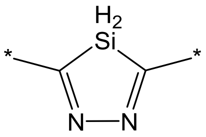
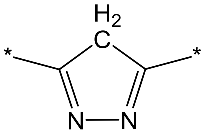
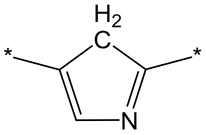
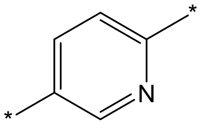
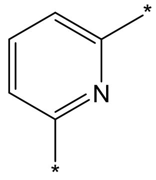


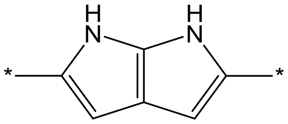
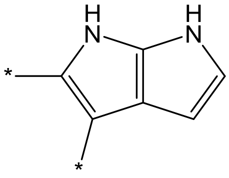
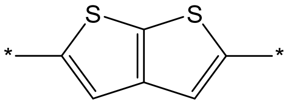
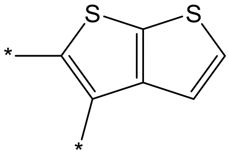
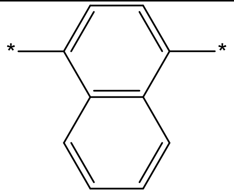
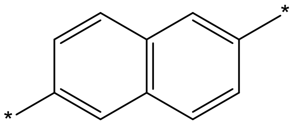
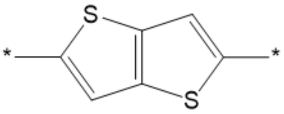
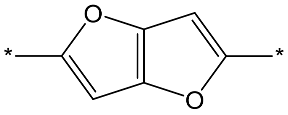
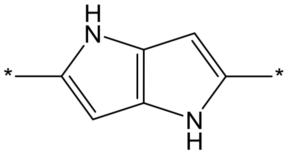
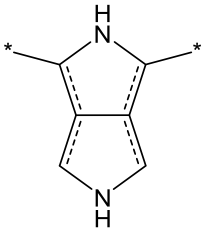
Figure S12. Plots of HOCO (filled) and LUCO (empty) energy levels against QSE$_{SC,CO}$ for the 179 copolymers. The blue and red symbols indicate aromatic and quinoidal orbitals, respectively.

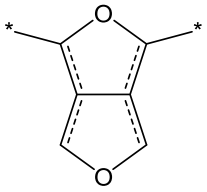
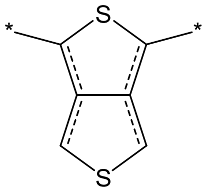
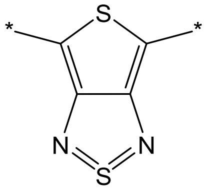
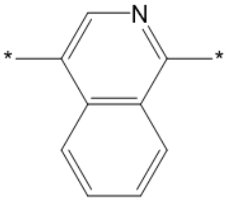
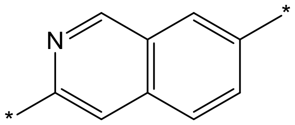
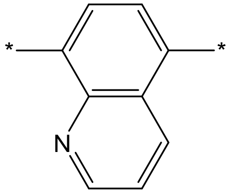
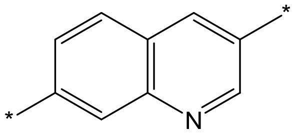
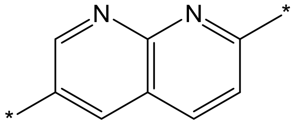
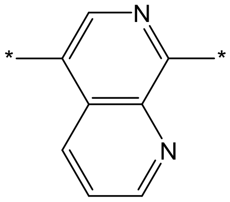
G. List of QSE

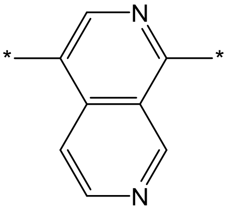
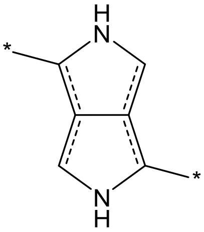
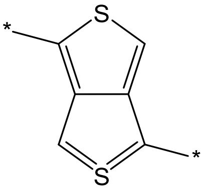
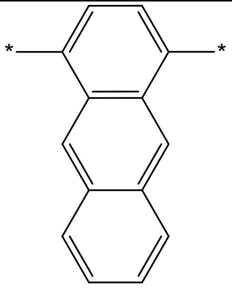
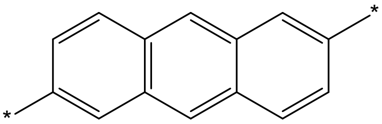
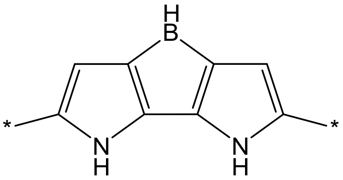
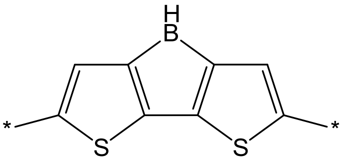
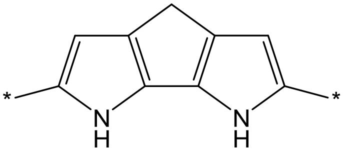
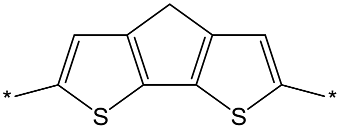
The chemical structures, SMILES, QSE, and size-corrected QSE (QSE$_{SC}$) of the 268 monomers calculated in this study are summarized in the table below. In the chemical structures and SMILES, * indicates linking sites.

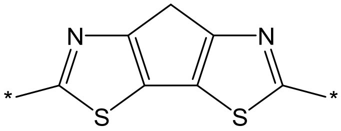
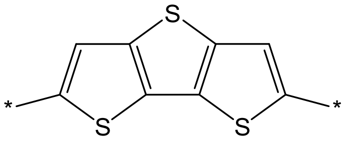
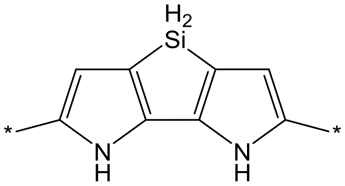
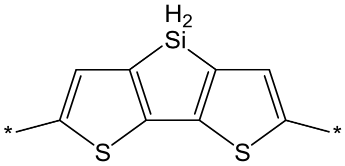
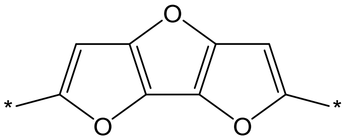
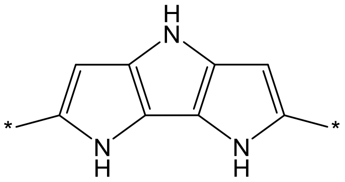
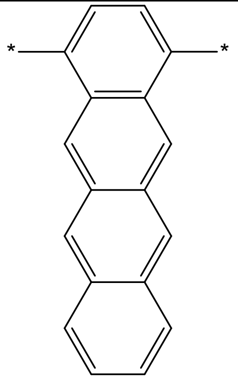
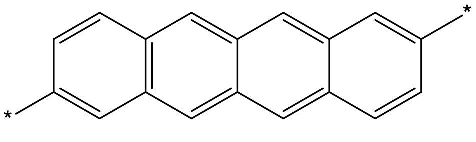
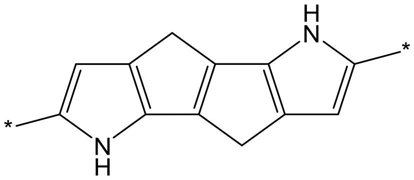
Chemical Structure	**SMILES**	**QSE**	**QSE$_{SC}$**
	[*]C1=CC=C([*])C=C1	23.62	11.81
	[*]C1=CC=CC([*])=C1	47.98	27.70
	[*]C1=C(F)C(F)=C([*])C(F)=C1F	26.44	13.22

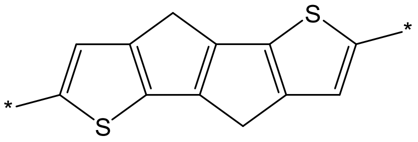
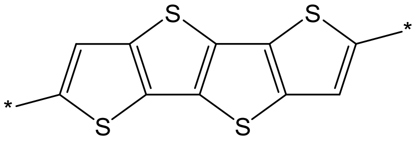
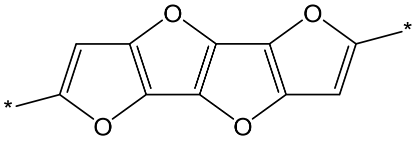
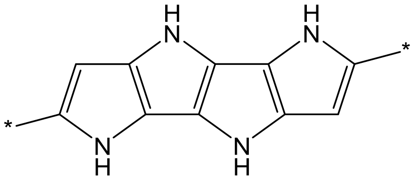
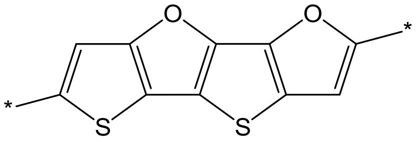
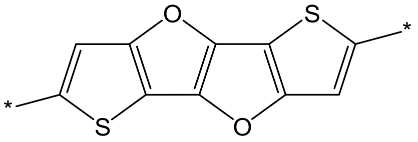
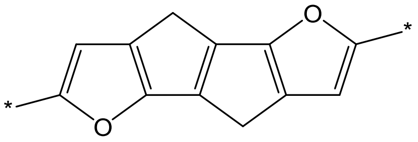
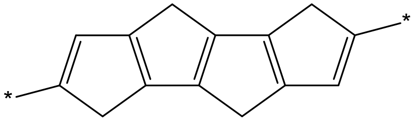
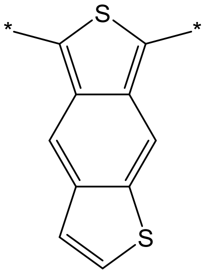
	[*]C1=CC=C(/C=C/[*])C=C1	21.73	8.87
	[*]C1=CN=C([*])S1	16.16	8.08
	[*]C1=CN=C([*])O1	17.29	8.64
	[*]C1=CN=C([*])N1	18.46	9.23
	[*]C1=NN=C([*])S1	25.22	12.61
	[*]C1=NN=C([*])O1	28.63	14.31
	[*]C1=NN=C([*])N1	29.58	14.79
	[*]C1=NN=C([*])[SiH2]1	5.59	2.79
	[*]C1=NN=C([*])C1	12.41	6.20
	[*]C1=CN=C([*])C1	3.41	1.70
	[*]C1=CC=C([*])C=N1	25.09	12.55
	[*]C1=CC=CC([*])=N1	49.98	28.86

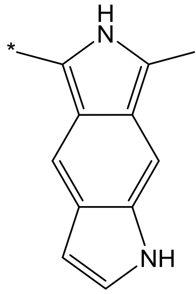
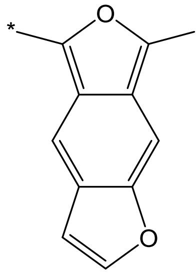
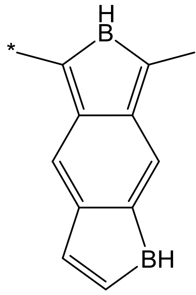
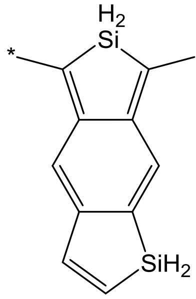
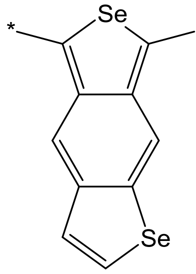
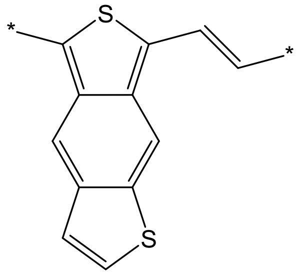
	[*]C1=CC(C=C([*])N2)=C2N1	27.94	12.49
	[*]C1=C([*])C(C=CN2)=C2N1	8.48	5.99
	[*]C1=CC(C=C([*])S2)=C2S1	47.50	21.24
	[*]C1=C([*])C(C=CS2)=C2S1	12.11	8.56
	[*]C1=CC=C([*])C2=C1C=CC=C2	18.45	9.22
	[*]C1=CC2=C(C=C1)C=C([*])C=C2	33.13	13.52
	[*]C1=CC(SC([*])=C2)=C2S1	16.61	6.78
	[*]C1=CC(OC([*])=C2)=C2O1	9.10	3.71
	[*]C1=CC(NC([*])=C2)=C2N1	10.88	4.44
	[*]c1c2cNcc2c([*])N1	-15.44	-7.72

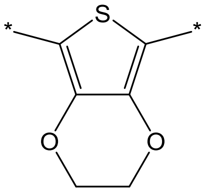
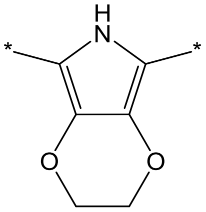
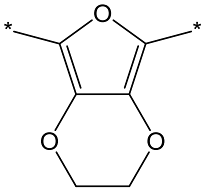
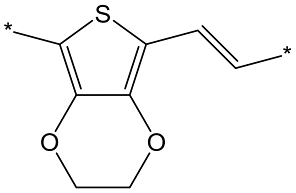
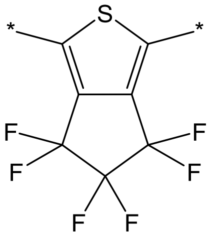
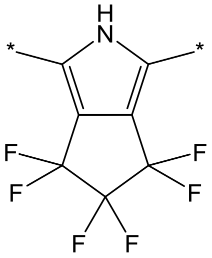
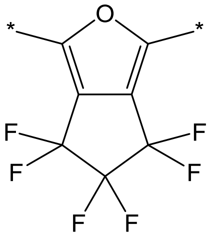
	[*]c1c2cOcc2c([*])O1	-22.90	-11.45
	[*]C1=C(C=S=C2)C2=C([*])S1	-16.37	-8.18
	[*]C1=C(N=S=N2)C2=C([*])S1	-12.21	-6.11
	[*]C1=CN=C([*])C2=C1C=CC=C2	19.45	9.72
	[*]C1=CC2=C(C=N1)C=C([*])C=C2	34.23	13.97
	[*]C1=CC=C([*])C2=C1N=CC=C2	17.70	8.85
	[*]C1=CC2=C(C=C1)C=C([*])C=N2	33.64	13.74
	[*]C1=CC2=C(N=C1)N=C([*])C=C2	35.44	14.47
	[*]C1=CN=C([*])C2=C1C=CC=N2	18.54	9.27

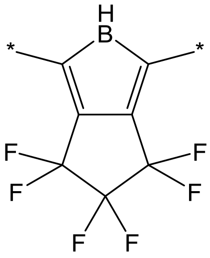
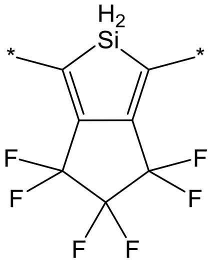
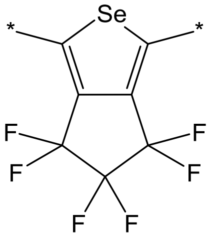
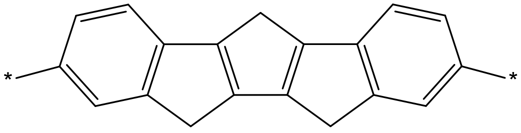
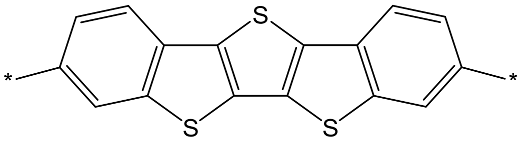
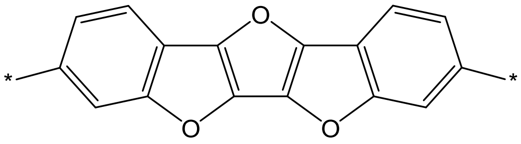
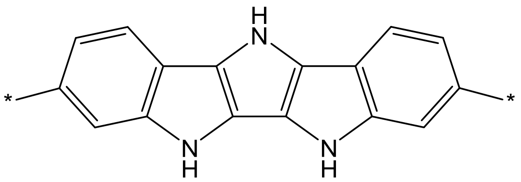
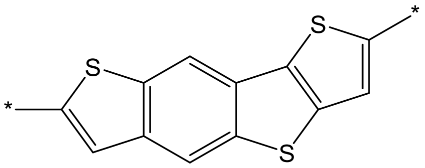
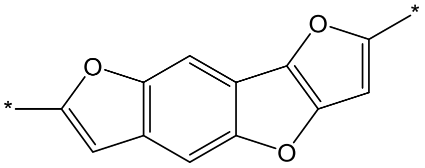
	[*]C1=CN=C([*])C2=C1C=CN=C2	19.70	9.85
	[*]c1c2cNc([*])c2cN1	3.39	1.70
	[*]C1=C(C=S=C2[*])C2=CS1	-2.44	-1.22
	[*]C1=CC=C([*])C2=C1C=C(C=CC=C3)C3=C2	15.49	7.74
	[*]C1=CC2=C(C=C1)C=C3C(C=CC([*])=C3)=C2	34.48	12.19
	[*]C(N1)=CC2=C1C(NC([*])=C3)=C3B2	18.05	7.37
	[*]C(S1)=CC2=C1C(SC([*])=C3)=C3B2	14.16	5.78
	[*]C(N1)=CC2=C1C(NC([*])=C3)=C3C2	15.82	5.59
	[*]C(S1)=CC2=C1C(SC([*])=C3)=C3C2	15.57	5.50

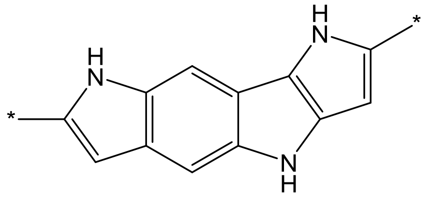
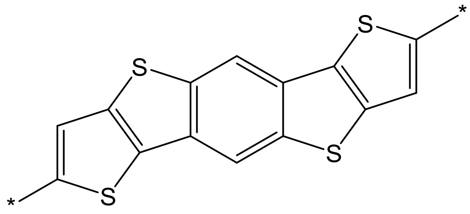
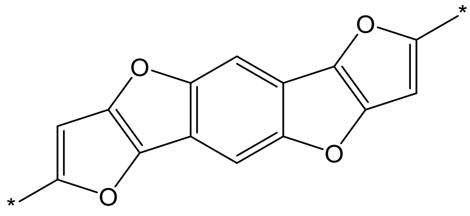
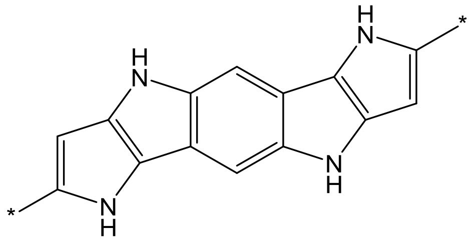
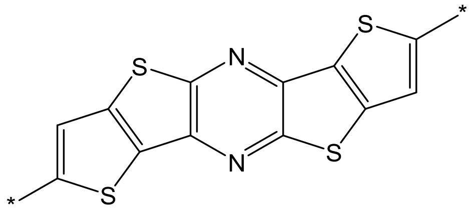
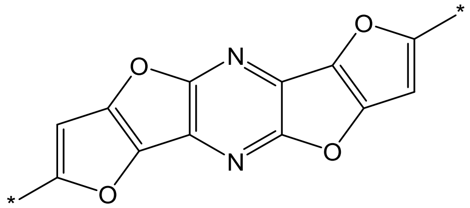
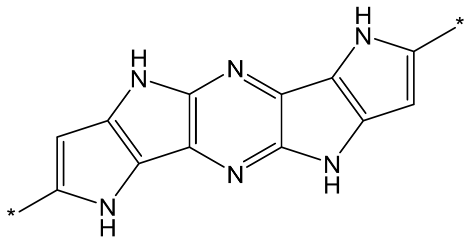
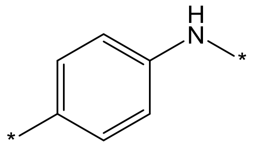
	[*]C(S1)=NC2=C1C(SC([*])=N3)=C3C2	16.83	5.95
	[*]C(S1)=CC2=C1C(SC([*])=C3)=C3S2	22.16	7.83
	[*]C(N1)=CC2=C1C(NC([*])=C3)=C3[SiH2]2	21.94	7.76
	[*]C(S1)=CC2=C1C(SC([*])=C3)=C3[SiH2]2	19.21	6.79
	[*]C(O1)=CC2=C1C(OC([*])=C3)=C3O2	13.38	4.73
	[*]C(N1)=CC2=C1C(NC([*])=C3)=C3N2	16.23	5.74
	[*]C1=CC=C([*])C2=C1C=C(C=C(C=C(C=CC=C3)C3=C4)C4=C2	14.07	7.03
	[*]C1=CC2=C(C=C1)C=C3C(C=C(C=C(C=CC([*])=C4)C4=C3)=C2	33.13	10.48
	[*]C(N1)=CC2=C1C(CC3=C4NC([*])=C3)=C4C2	14.63	4.63

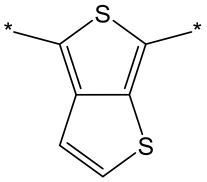
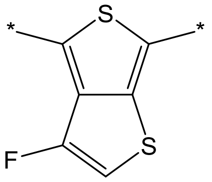
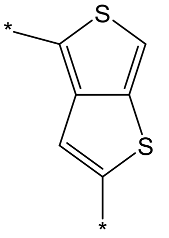
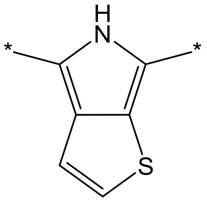
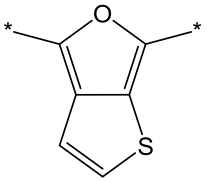
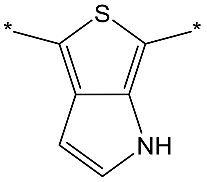
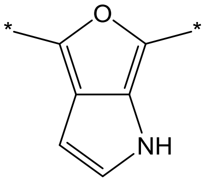
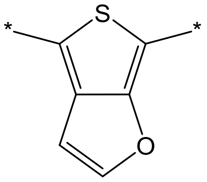
	[*]C(S1)=CC2=C1C(CC3=C4SC([*])=C3)=C4C2	13.94	4.41
	[*]C(S1)=CC2=C1C(SC3=C4SC([*])=C3)=C4S2	27.45	8.68
	[*]C(O1)=CC2=C1C(OC3=C4OC([*])=C3)=C4O2	16.51	5.22
	[*]C(N1)=CC2=C1C(NC3=C4NC([*])=C3)=C4N2	19.82	6.27
	[*]C(S1)=CC2=C1C(SC3=C4OC([*])=C3)=C4O2	23.32	7.37
	[*]C(S1)=CC2=C1C(OC3=C4SC([*])=C3)=C4O2	20.44	6.46
	[*]C(O1)=CC2=C1C(CC3=C4OC([*])=C3)=C4C2	10.56	3.34
	[*]C(C1)=CC2=C1C(CC3=C4CC([*])=C3)=C4C2	-5.91	-1.87
	[*]C1=C(C=C(C=CS2)C2=C3)C3=C([*])S1	-6.22	-3.11

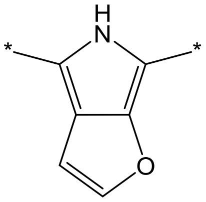
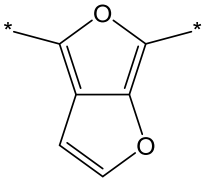
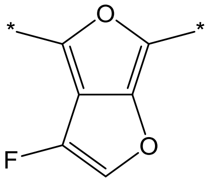
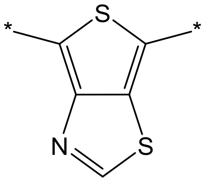
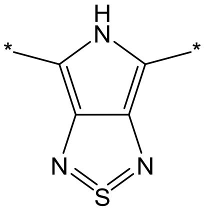
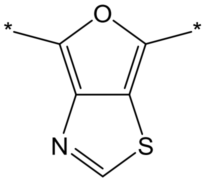
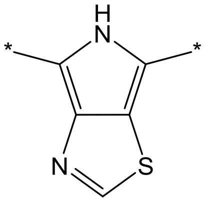
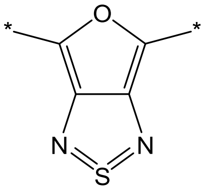
	[*]C1=C(C=C(C=CN2)C2=C3)C3=C([*])N1	-8.03	-4.01
	[*]C1=C(C=C(C=CO2)C2=C3)C3=C([*])O1	-9.53	-4.77
	[*]C1=C(C=C(C=CB2)C2=C3)C3=C([*])B1	-20.64	-10.32
	[*]C1=C(C=C(C=C[SiH2]2)C2=C3)C3=C([*])[SiH2]1	-19.72	-9.86
	[*]C1=C(C=C(C=C[Se]2)C2=C3)C3=C([*])[Se]1	-8.57	-4.28
	[*]C1=C(C=C(C=CS2)C2=C3)C3=C(/C=C/[*])S1	-7.25	-2.96

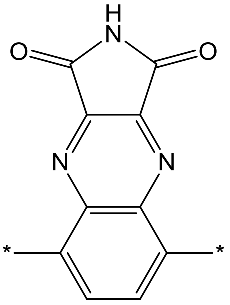
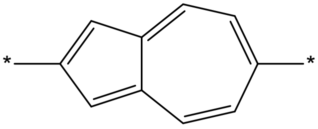
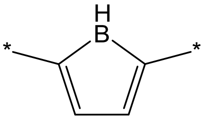
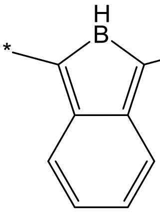
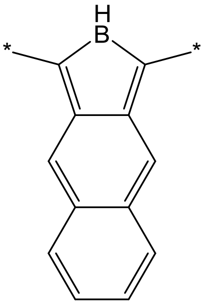
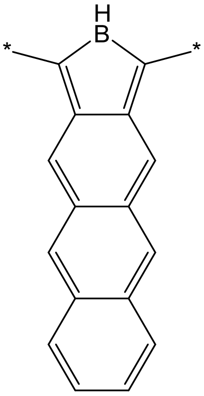
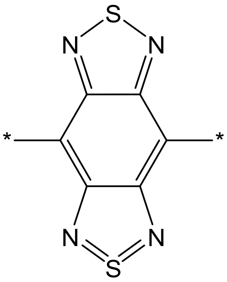
	[*]C1=C(OCCO2)C2=C([*])S1	8.12	4.06
	[*]C1=C(OCCO2)C2=C([*])N1	6.22	3.11
	[*]C1=C(OCCO2)C2=C([*])O1	4.87	2.43
	[*]C1=C(OCCO2)C2=C(/C=C/[*])S1	6.75	2.76
	[*]C1=C(C(F)(F)C(F)(F)C2(F)F)C2=C([*])S1	14.94	7.47
	[*]C1=C(C(F)(F)C(F)(F)C2(F)F)C2=C([*])N1	18.01	9.00
	[*]C1=C(C(F)(F)C(F)(F)C2(F)F)C2=C([*])O1	14.42	7.21

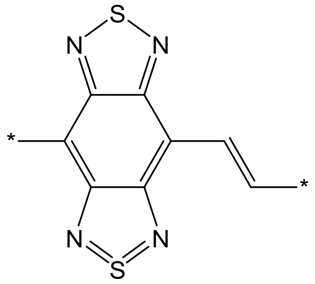
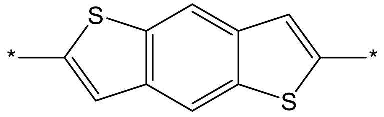
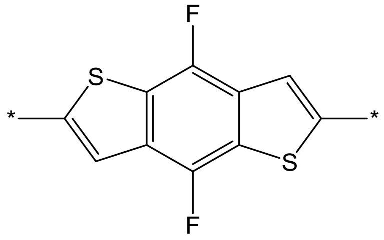
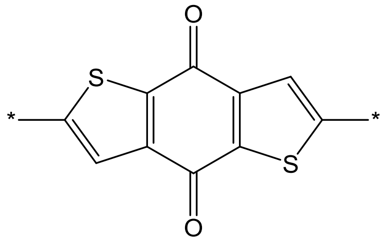
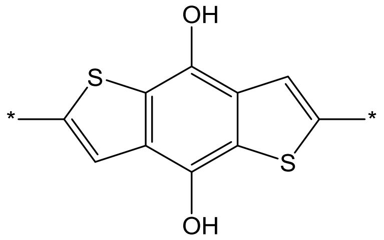
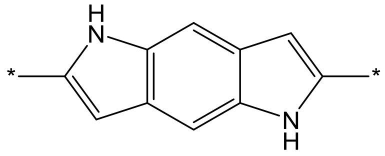
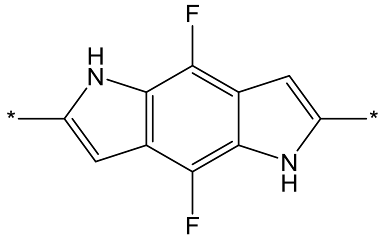
	[*]C1=C(C(F)(F)C(F)(F)C2(F)F)C2=C([*])B1	-14.14	-10.00
	[*]C1=C(C(F)(F)C(F)(F)C2(F)F)C2=C([*])[SiH2]1	-1.71	-0.86
	[*]C1=C(C(F)(F)C(F)(F)C2(F)F)C2=C([*])[Se]1	12.25	6.12
	[*]C(C=C1)=CC2=C1C3=C(C2)C4=C(C(C=CC([*])=C5)=C5C4)C3	34.91	10.08
	[*]C(C=C1)=CC2=C1C3=C(S2)C4=C(C(C=CC([*])=C5)=C5S4)S3	39.82	11.49
	[*]C(C=C1)=CC2=C1C3=C(O2)C4=C(C(C=CC([*])=C5)=C5O4)O3	38.22	11.03
	[*]C(C=C1)=CC2=C1C3=C(N2)C4=C(C(C=CC([*])=C5)=C5N4)N3	48.40	13.97
	[*]C1=CC2=C(S1)C=C3C(SC4=C3SC([*])=C4)=C2	30.73	9.72
	[*]C1=CC2=C(O1)C=C3C(OC4=C3OC([*])=C4)=C2	26.65	8.43

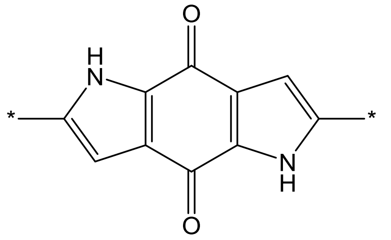
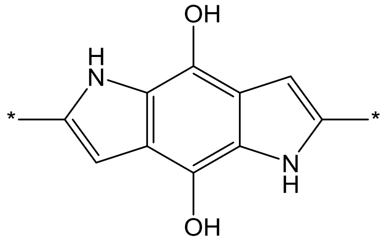
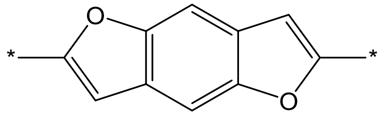
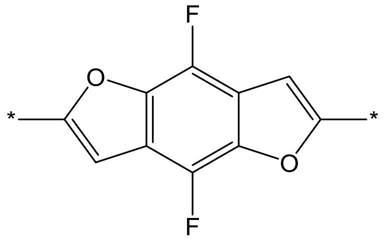
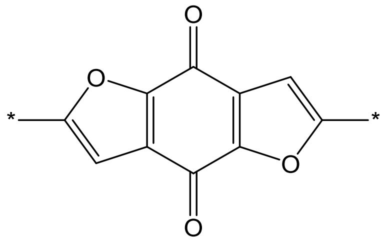
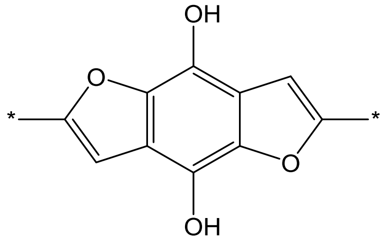
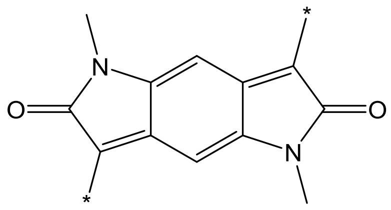
	[*]C1=CC2=C(N1)C=C3C(NC4=C3NC([*])=C4)=C2	26.78	8.47
	[*]C(S1)=CC2=C1C3=CC(SC4=C5SC([*])=C4)=C5C=C3S2	31.07	8.97
	[*]C(O1)=CC2=C1C3=CC(OC4=C5OC([*])=C4)=C5C=C3O2	25.69	7.42
	[*]C(N1)=CC2=C1C3=CC(NC4=C5NC([*])=C4)=C5C=C3N2	26.12	7.54
	[*]C(S1)=CC2=C1C3=NC(SC4=C5SC([*])=C4)=C5N=C3S2	30.67	8.85
	[*]C(O1)=CC2=C1C3=NC(OC4=C5OC([*])=C4)=C5N=C3O2	24.31	7.02
	[*]C(N1)=CC2=C1C3=NC(NC4=C5NC([*])=C4)=C5N=C3N2	25.14	7.26
	[*]C1=CC=C(N[*])C=C1	43.53	17.77

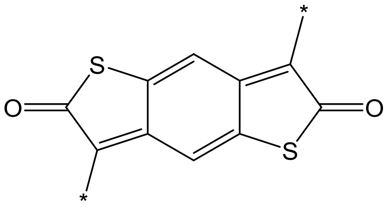
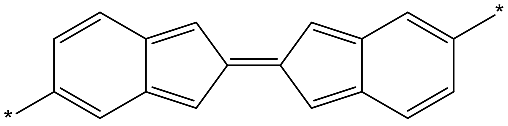
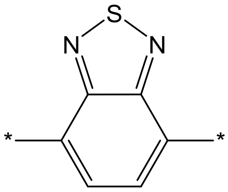
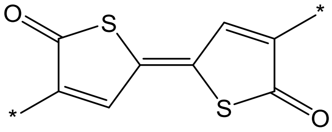
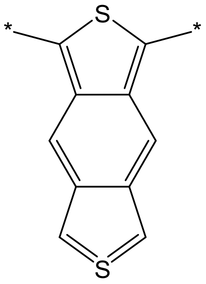
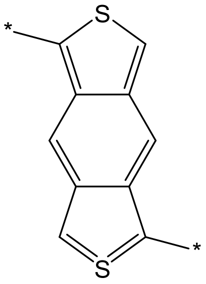
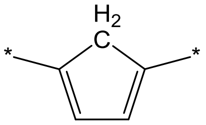
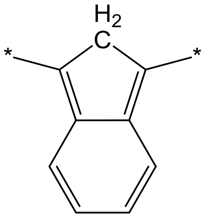
	[*]C1=C(C=CS2)C2=C([*])S1	3.51	1.75
	[*]C1=C(C(F)=CS2)C2=C([*])S1	4.07	2.03
	[*]C1=C(C=C([*])S2)C2=CS1	17.17	8.59
	[*]C1=C(C=CS2)C2=C([*])N1	3.62	1.81
	[*]C1=C(C=CS2)C2=C([*])O1	1.19	0.59
	[*]C1=C(C=CN2)C2=C([*])S1	-1.15	-0.58
	[*]C1=C(C=CN2)C2=C([*])O1	-4.04	-2.02
	[*]C1=C(C=CO2)C2=C([*])S1	3.28	1.64

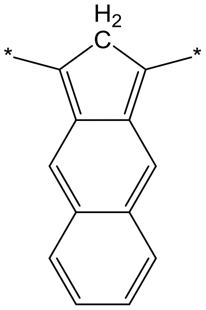
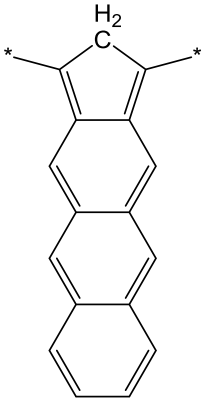
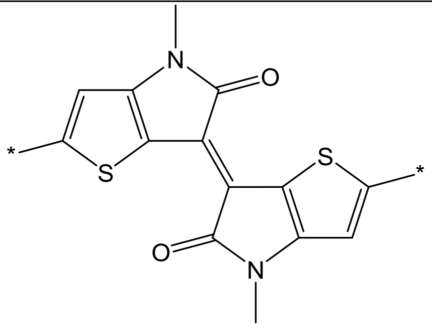
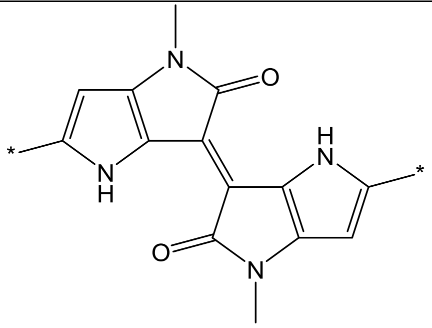
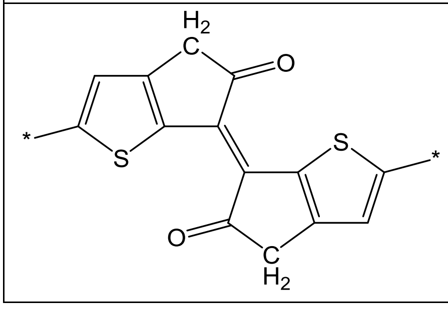
	[*]C1=C(C=CO2)C2=C([*])N1	2.71	1.35
	[*]C1=C(C=CO2)C2=C([*])O1	0.72	0.36
	[*]C1=C(C(F)=CO2)C2=C([*])O1	1.06	0.53
	[*]C1=C(N=CS2)C2=C([*])S1	5.34	2.67
	[*]C1=C(N=S=N2)C2=C([*])N1	-9.08	-4.54
	[*]C1=C(N=CS2)C2=C([*])O1	3.22	1.61
	[*]C1=C(N=CS2)C2=C([*])N1	5.90	2.95
	[*]C1=C(N=S=N2)C2=C([*])O1	-15.74	-7.87

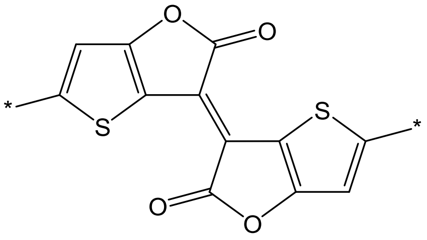
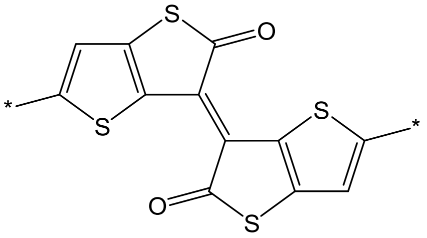
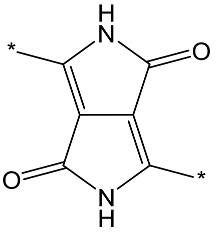
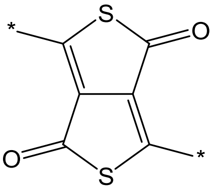
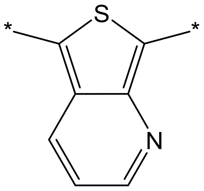
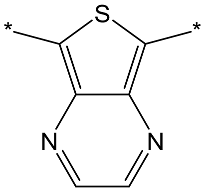
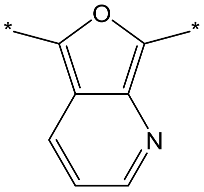
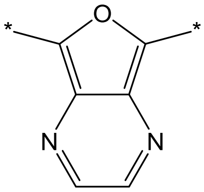
	O=C1C2=NC(C([*])=CC=C3[*])=C3N=C2C(N1)=O	18.14	9.07
	[*]C1=CC2=CC=C([*])C=CC2=C1	14.71	6.00
	[*]C1=CC=C([*])B1	-11.40	-5.70
	[*]C1=C(C=CC=C2)C2=C([*])B1	-25.71	-12.85
	[*]C1=C(C=C(C=CC=C2)C2=C3)C3=C([*])B1	-22.02	-11.01
	[*]C1=C(C=C(C=C(C=CC=C2)C2=C3)C3=C4)C4=C([*])B1	-18.75	-9.38
	[*]C1=C2C(N=S=N2)=C([*])C3=NSN=C31	-10.69	-5.34

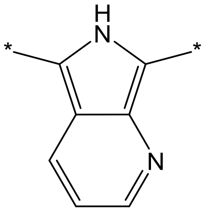
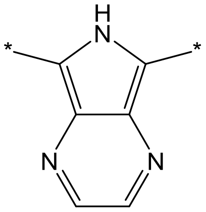
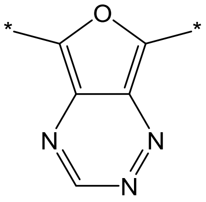
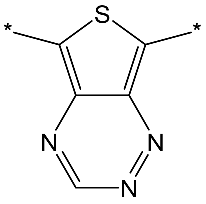
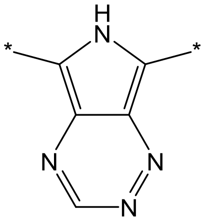
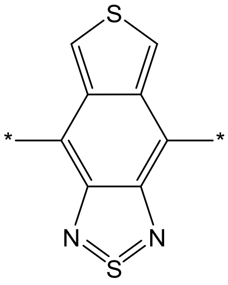
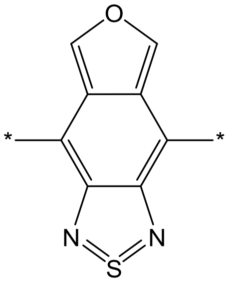
	[*]C1=C(N=S=N2)C2=C(/C=C/[*])C3=NSN=C31	-12.27	-5.01
	[*]C1=CC2=C(S1)C=C3C(SC([*])=C3)=C2	31.35	11.08
	[*]C1=CC2=C(S1)C(F)=C3C(SC([*])=C3)=C2F	32.77	11.59
	[*]C1=CC(C(C2=C3C=C([*])S2)=O)=C(S1)C3=O	35.63	12.60
	[*]C1=CC2=C(S1)C(O)=C3C(SC([*])=C3)=C2O	29.73	10.51
	[*]C1=CC2=C(N1)C=C3C(NC([*])=C3)=C2	28.02	9.91
	[*]C1=CC2=C(N1)C(F)=C3C(NC([*])=C3)=C2F	30.09	10.64

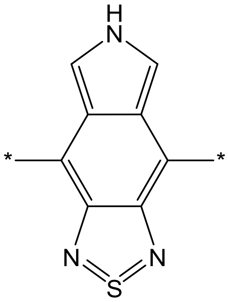
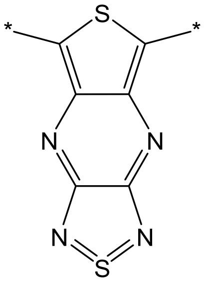
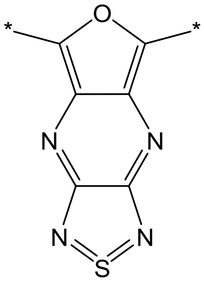
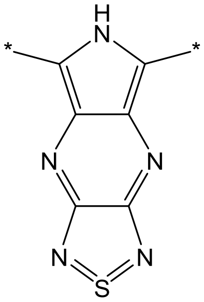
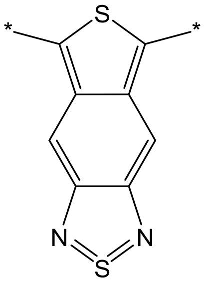
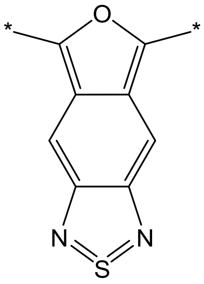
	[*]C1=CC(C(C2=C3C=C([*])N2)=O)=C(N1)C3=O	37.31	13.19
	[*]C1=CC2=C(N1)C(O)=C3C(NC([*])=C3)=C2O	32.13	11.36
	[*]C1=CC2=C(O1)C=C3C(OC([*])=C3)=C2	27.07	9.57
	[*]C1=CC2=C(O1)C(F)=C3C(OC([*])=C3)=C2F	31.83	11.25
	[*]C1=CC(C(C2=C3C=C([*])O2)=O)=C(O1)C3=O	36.19	12.79
	[*]C1=CC2=C(O1)C(O)=C3C(OC([*])=C3)=C2O	26.21	9.27
	O=C1N(C)C(C(C=C2N3C)=C1[*])=CC2=C([*])C3=O	-7.61	-3.11

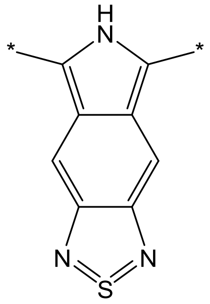
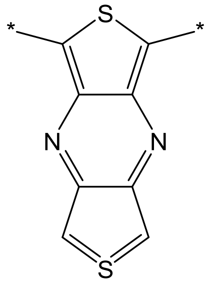
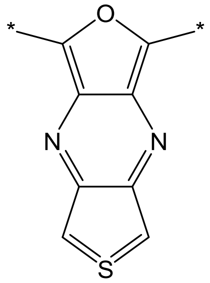
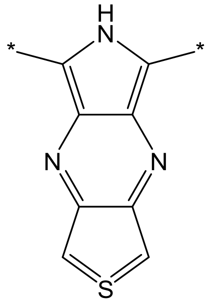
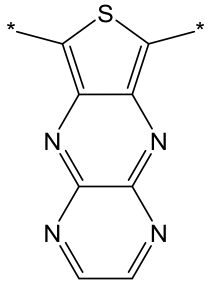
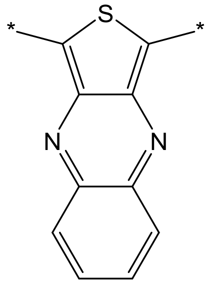
	O=C1SC(C(C=C2S3)=C1[*])=CC2=C([*])C3=O	-8.14	-3.32
	[*]C1=CC(C(C=C1)=C/2)=CC2=C3C=C(C=CC([*])=C4)C4=C/3	-15.98	-5.05
	[*]C1=CC=C([*])C2=NSN=C21	13.20	6.60
	O=C1C([*])=C/C(S1)=C2SC(C([*])=C¥2)=O	10.58	4.32
	[*]C1=C(C=C(C=S=C2)C2=C3)C3=C([*])S1	-16.51	-8.25
	[*]C1=C(C=C(C=S=C2[*])C2=C3)C3=CS1	2.53	1.03
	[*]C1=CC=C([*])C1	0.42	0.21
	[*]C1=C(C=CC=C2)C2=C([*])C1	-19.88	-9.94

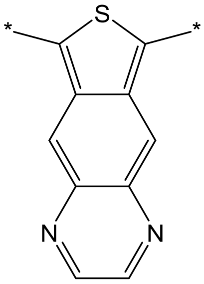
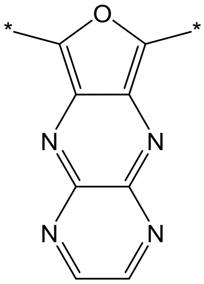
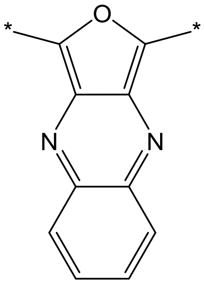
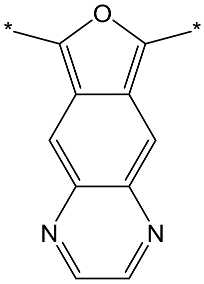
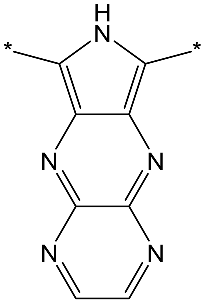
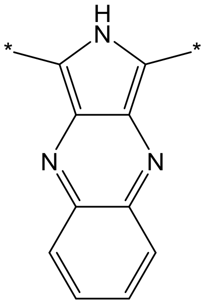
	[*]C1=C(C=C(C=CC=C2)C2=C3)C3=C([*])C1	-26.53	-13.27
	[*]C1=C(C=C(C=C(C=CC=C2)C2=C3)C3=C4)C4=C([*])C1	-25.35	-12.68
	O=C1/C(C2=C(C=C([*])S2)N1C)=C3C(N(C)C4=C/3SC([*])=C4)=O	7.10	2.24
	O=C1/C(C2=C(C=C([*])N2)N1C)=C3C(N(C)C4=C/3NC([*])=C4)=O	3.86	1.22
	O=C1/C(C2=C(C=C([*])S2)C1)=C3C(CC4=C/3SC([*])=C4)=O	12.00	3.79

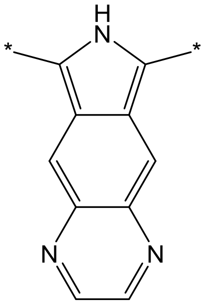
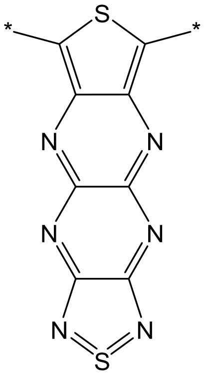
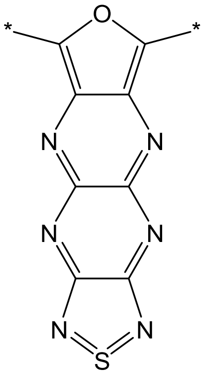
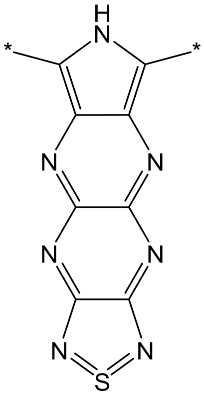
	O=C1/C(C2=C(C=C([*])S2)O1)=C3C(OC4=C/3SC([*])=C4)=O	7.75	2.45
	O=C1/C(C2=C(C=C([*])S2)S1)=C3C(SC4=C/3SC([*])=C4)=O	8.97	2.84
	[*]C1=C2C(C(N1)=O)=C([*])NC2=O	2.91	1.45
	[*]C1=C2C(C(S1)=O)=C([*])SC2=O	5.76	2.88
	[*]C1=C(C=CC=N2)C2=C([*])S1	-2.31	-1.16
	[*]C1=C(N=CC=N2)C2=C([*])S1	-1.30	-0.65
	[*]C1=C(C=CC=N2)C2=C([*])O1	-4.82	-2.41
	[*]C1=C(N=CC=N2)C2=C([*])O1	-3.56	-1.78

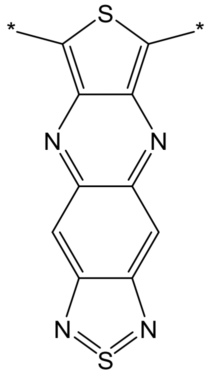
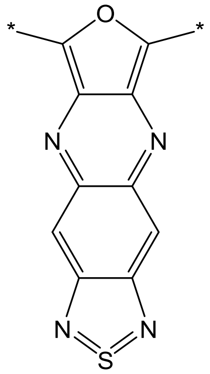
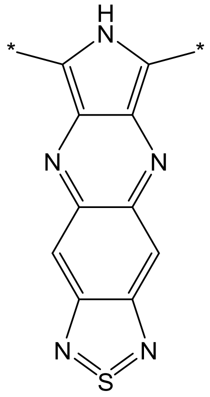
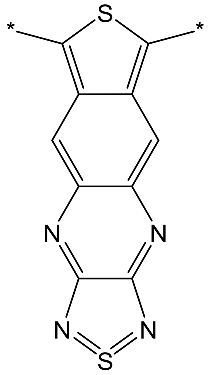
	[*]C1=C(C=CC=N2)C2=C([*])N1	-0.38	-0.19
	[*]C1=C(N=CC=N2)C2=C([*])N1	1.36	0.68
	[*]C1=C(N=CN=N2)C2=C([*])O1	-4.10	-2.05
	[*]C1=C(N=CN=N2)C2=C([*])S1	-1.84	-0.92
	[*]C1=C(N=CN=N2)C2=C([*])N1	1.86	0.93
	[*]C1=C(N=S=N2)C2=C([*])C3=CSC=C31	-9.98	-4.99
	[*]C1=C(N=S=N2)C2=C([*])C3=COC=C31	-12.32	-6.16

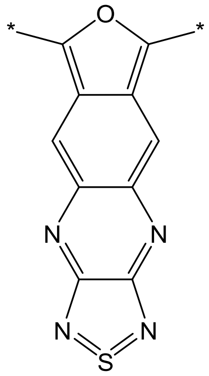
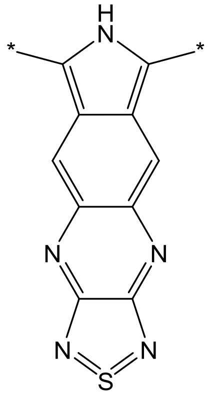
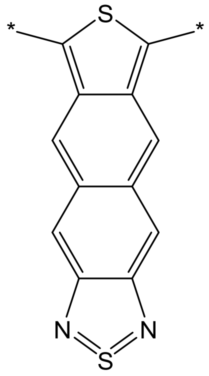
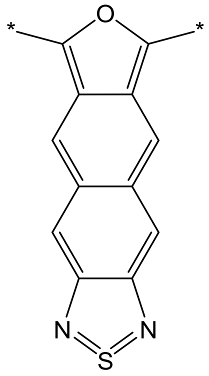
	[*]C1=C(N=S=N2)C2=C([*])C3=CNC=C31	-9.45	-4.73
	[*]C1=C(N=C(N=S=N2)C2=N3)C3=C([*])S1	-11.05	-5.53
	[*]C1=C(N=C(N=S=N2)C2=N3)C3=C([*])O1	-14.06	-7.03
	[*]C1=C(N=C(N=S=N2)C2=N3)C3=C([*])N1	-7.32	-3.66
	[*]C1=C(C=C(N=S=N2)C2=C3)C3=C([*])S1	-11.90	-5.95
	[*]C1=C(C=C(N=S=N2)C2=C3)C3=C([*])O1	-15.81	-7.91

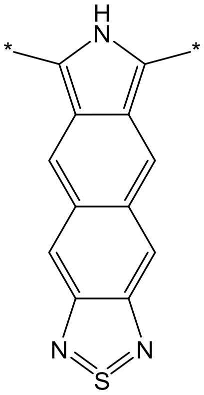
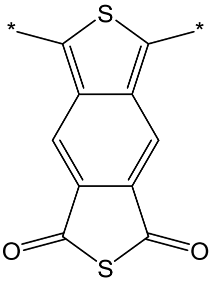
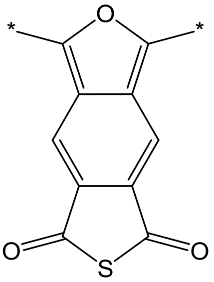
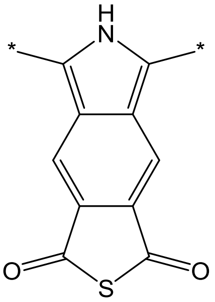
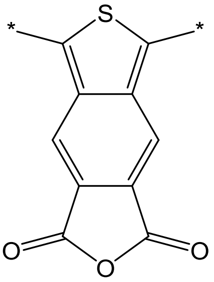
	[*]C1=C(C=C(N=S=N2)C2=C3)C3=C([*])N1	-11.15	-5.58
	[*]C1=C(N=C(C=S=C2)C2=N3)C3=C([*])S1	-12.30	-6.15
	[*]C1=C(N=C(C=S=C2)C2=N3)C3=C([*])O1	-15.24	-7.62
	[*]C1=C(N=C(C=S=C2)C2=N3)C3=C([*])N1	-10.03	-5.02
	[*]C1=C(N=C(N=CC=N2)C2=N3)C3=C([*])S1	-7.84	-3.92
	[*]C1=C(N=C(C=CC=C2)C2=N3)C3=C([*])S1	-8.74	-4.37

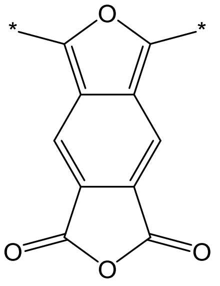
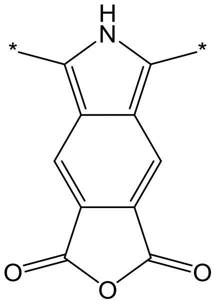
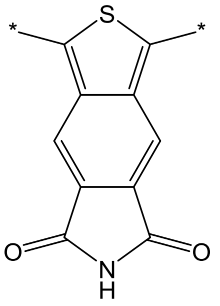
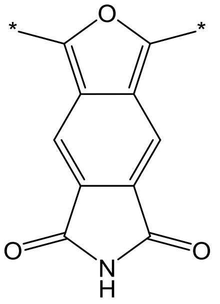
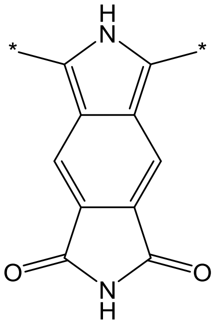
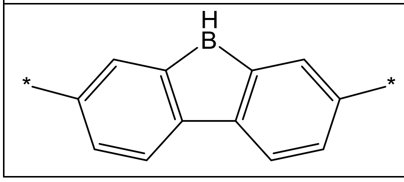
	[*]C1=C(C=C(N=CC=N2)C2=C3)C3=C([*])S1	-8.77	-4.39
	[*]C1=C(N=C(N=CC=N2)C2=N3)C3=C([*])O1	-10.91	-5.46
	[*]C1=C(N=C(C=CC=C2)C2=N3)C3=C([*])O1	-11.89	-5.95
	[*]C1=C(C=C(N=CC=N2)C2=C3)C3=C([*])O1	-12.40	-6.20
	[*]C1=C(N=C(N=CC=N2)C2=N3)C3=C([*])N1	-3.92	-1.96
	[*]C1=C(N=C(C=CC=C2)C2=N3)C3=C([*])N1	-5.49	-2.75

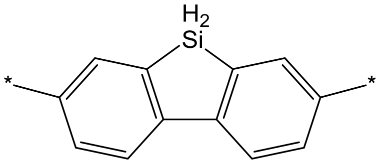
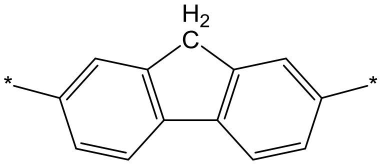
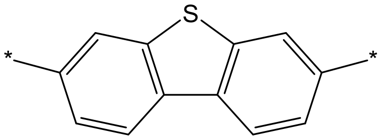
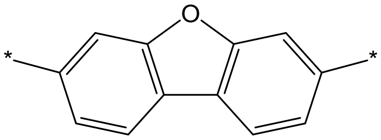
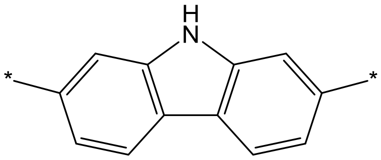
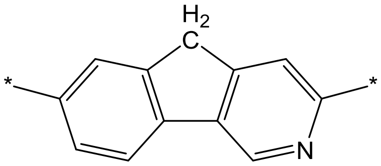
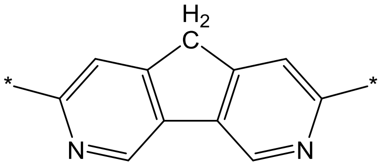
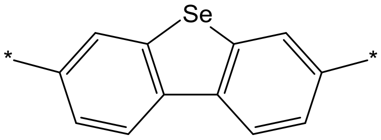
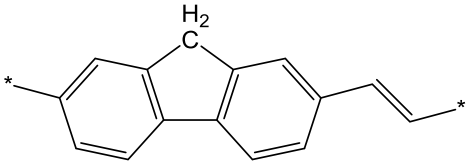
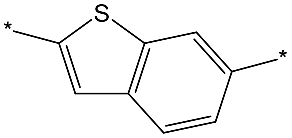
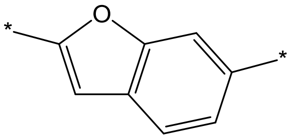
	[*]C1=C(C=C(N=CC=N2)C2=C3)C3=C([*])N1	-6.94	-3.47
	[*]C1=C(N=C(N=C(N=S=N2)C2=N3)C3=N4)C4=C([*])S1	-11.14	-5.57
	[*]C1=C(N=C(N=C(N=S=N2)C2=N3)C3=N4)C4=C([*])O1	-13.69	-6.85
	[*]C1=C(N=C(N=C(N=S=N2)C2=N3)C3=N4)C4=C([*])N1	-7.28	-3.64

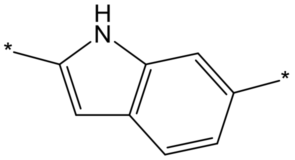
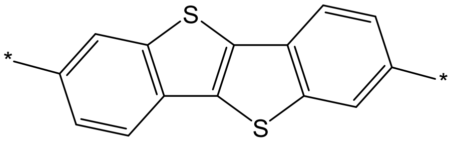
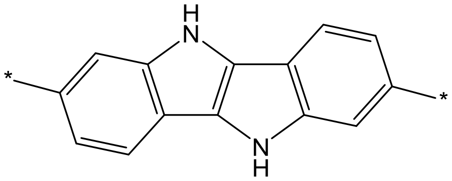
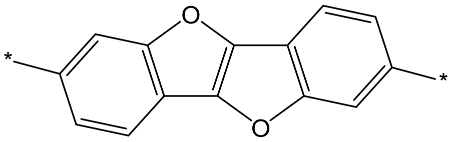
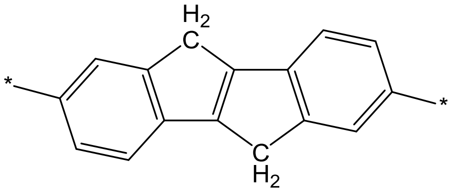
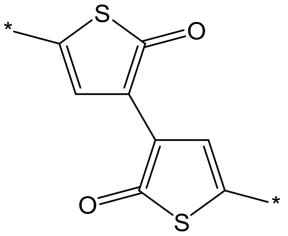
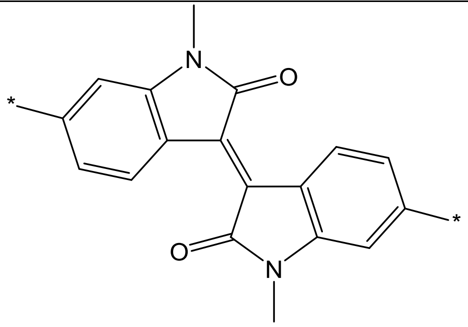
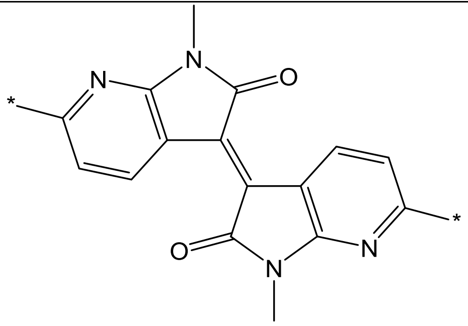
	[*]C1=C(N=C(C=C(N=S=N2)C2=C3)C3=N4)C4=C([*])S1	-10.63	-5.32
	[*]C1=C(N=C(C=C(N=S=N2)C2=C3)C3=N4)C4=C([*])O1	-13.23	-6.62
	[*]C1=C(N=C(C=C(N=S=N2)C2=C3)C3=N4)C4=C([*])N1	-8.03	-4.02
	[*]C1=C(C=C(N=C(N=S=N2)C2=N3)C3=C4)C4=C([*])S1	-9.74	-4.87

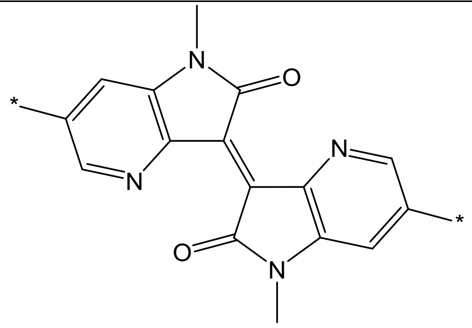
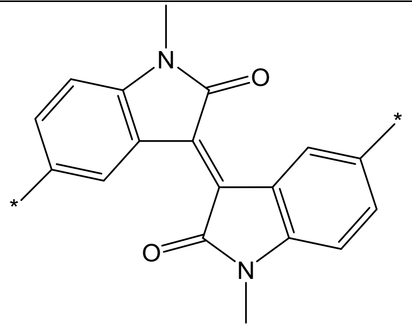
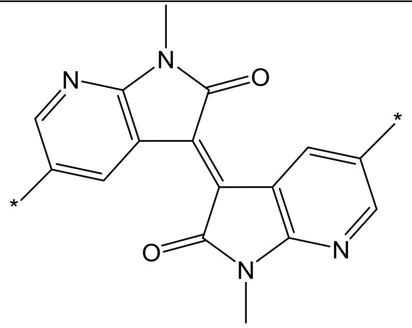
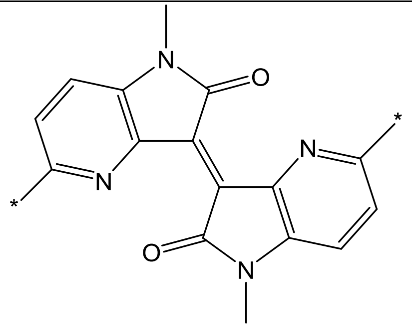
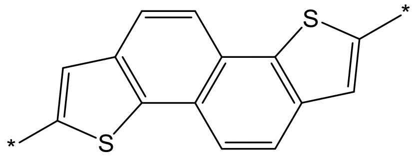
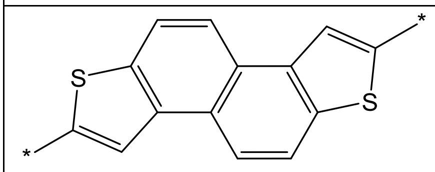
	[*]C1=C(C=C(N=C(N=S=N2)C2=N3)C3=C4)C4=C([*])O1	-12.82	-6.41
	[*]C1=C(C=C(N=C(N=S=N2)C2=N3)C3=C4)C4=C([*])N1	-11.61	-5.81
	[*]C1=C(C=C(C=C(N=S=N2)C2=C3)C3=C4)C4=C([*])S1	-10.24	-5.12
	[*]C1=C(C=C(C=C(N=S=N2)C2=C3)C3=C4)C4=C([*])O1	-13.62	-6.81

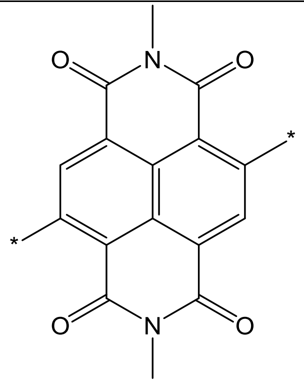
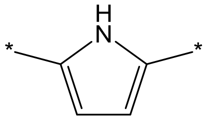
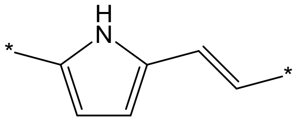
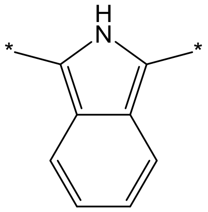
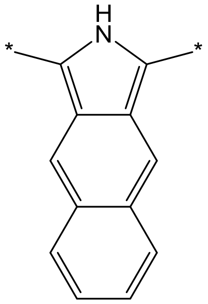
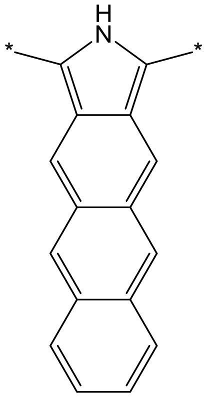
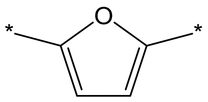
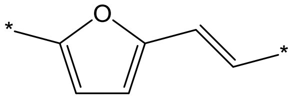
	[*]C1=C(C=C(C=C(N=S=N2)C2=C3)C3=C4)C4=C([*])N1	-9.90	-4.95
	[*]C1=C(C=C(C(SC2=O)=O)C2=C3)C3=C([*])S1	0.89	0.44
	[*]C1=C(C=C(C(SC2=O)=O)C2=C3)C3=C([*])O1	-1.41	-0.71
	[*]C1=C(C=C(C(SC2=O)=O)C2=C3)C3=C([*])N1	3.71	1.85
	[*]C1=C(C=C(C(OC2=O)=O)C2=C3)C3=C([*])S1	0.94	0.47

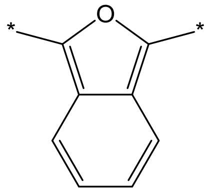
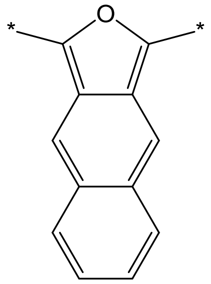
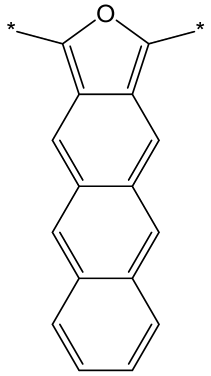
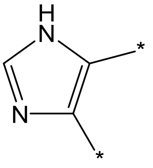
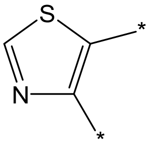
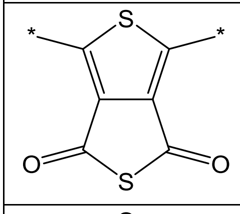
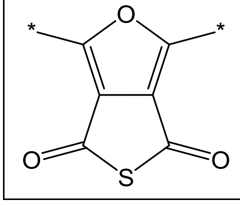
	[*]C1=C(C=C(C(OC2=O)=O)C2=C3)C3=C([*])O1	-1.45	-0.73
	[*]C1=C(C=C(C(OC2=O)=O)C2=C3)C3=C([*])N1	3.69	1.84
	[*]C1=C(C=C(C(NC2=O)=O)C2=C3)C3=C([*])S1	0.67	0.33
	[*]C1=C(C=C(C(NC2=O)=O)C2=C3)C3=C([*])O1	-1.73	-0.87
	[*]C1=C(C=C(C(NC2=O)=O)C2=C3)C3=C([*])N1	2.97	1.48
	[*]C(C=C1)=CC2=C1C(C=CC([*])=C3)=C3B2	39.73	16.22

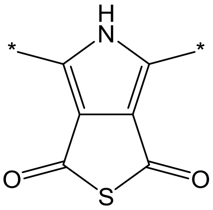
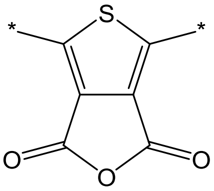
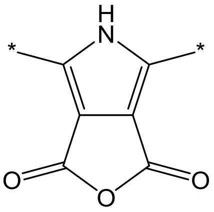
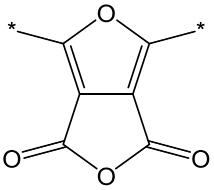
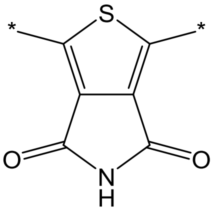
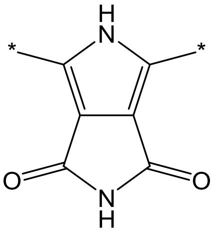
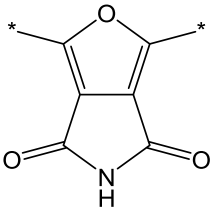
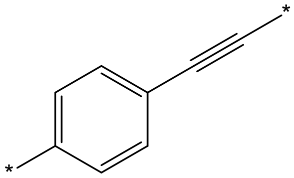
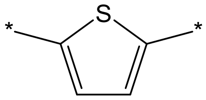
	[*]C(C=C1)=CC2=C1C(C=CC([*])=C3)=C3[SiH2]2	37.08	13.11
	[*]C(C=C1)=CC2=C1C(C=CC([*])=C3)=C3C2	36.65	12.96
	[*]C(C=C1)=CC2=C1C(C=CC([*])=C3)=C3S2	38.24	13.52
	[*]C(C=C1)=CC2=C1C(C=CC([*])=C3)=C3O2	37.78	13.36
	[*]C(C=C1)=CC2=C1C(C=CC([*])=C3)=C3N2	37.68	13.32
	[*]C(C=C1)=CC2=C1C(C=NC([*])=C3)=C3C2	38.63	13.66
	[*]C(N=C1)=CC2=C1C(C=NC([*])=C3)=C3C2	40.64	14.37
	[*]C(C=C1)=CC2=C1C(C=CC([*])=C3)=C3[Se]2	37.96	13.42
	[*]C(C=C1)=CC2=C1C(C=CC(/C=C/[*])=C3)=C3C2	39.48	12.48
	[*]C1=CC2=C(C=C1)C=C([*])S2	28.47	11.62
	[*]C1=CC2=C(C=C1)C=C([*])O2	27.53	11.24

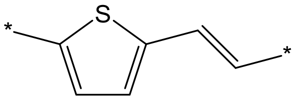
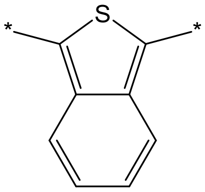
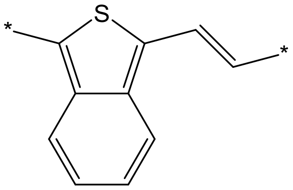
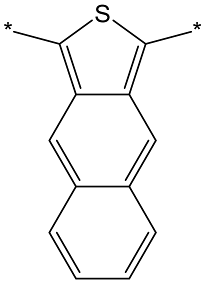
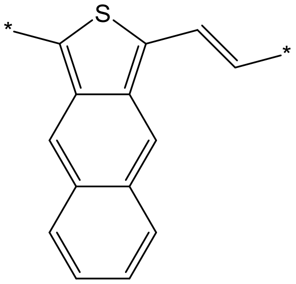
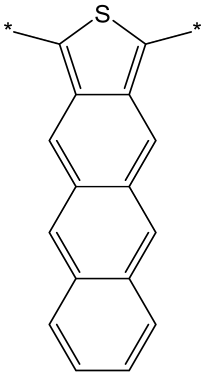
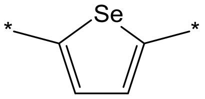
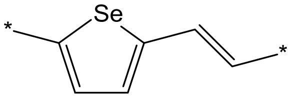
	[*]C1=CC2=C(C=C1)C=C([*])N2	28.13	11.48
	[*]C(C=C1)=CC2=C1C(SC3=C4C=CC([*])=C3)=C4S2	48.36	15.29
	[*]C(C=C1)=CC2=C1C(NC3=C4C=CC([*])=C3)=C4N2	37.21	11.77
	[*]C(C=C1)=CC2=C1C(OC3=C4C=CC([*])=C3)=C4O2	37.44	11.84
	[*]C(C=C1)=CC2=C1C(CC3=C4C=CC([*])=C3)=C4C2	41.02	12.97
	O=C(SC([*])=C1)=C1C(C=C([*])S2)=C2=O	-1.30	-0.53
	O=C1/C(C2=C(C=C([*])C=C2)N1C)=C3C(N(C)C4=C/3C=CC([*])=C4)=O	31.20	9.87
	O=C1/C(C2=C(N=C([*])C=C2)N1C)=C3C(N(C)C4=C/3C=CC([*])=N4)=O	34.62	10.95

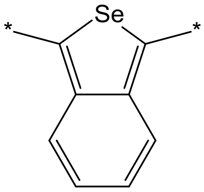
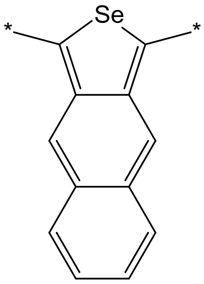
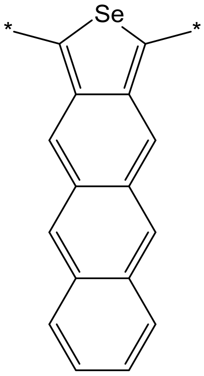
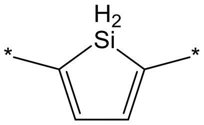
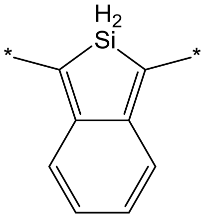
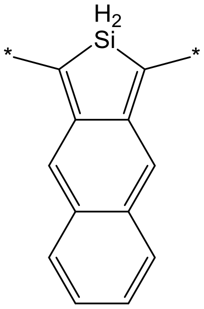
	O=C1/C(C2=C(C=C([*])C=N2)N1C)=C3C(N(C)C4=C/3N=CC([*])=C4)=O	25.52	8.07
	O=C1/C(C2=C(C=CC([*])=C2)N1C)=C3C(N(C)C4=C/3C=C([*])C=C4)=O	41.54	14.69
	O=C1/C(C2=C(N=CC([*])=C2)N1C)=C3C(N(C)C4=C/3C=C([*])C=N4)=O	42.89	15.16
	O=C1/C(C2=C(C=CC([*])=N2)N1C)=C3C(N(C)C4=C/3N=C([*])C=C4)=O	43.72	15.46
	[*]C(S1)=CC2=C1C3=C(C=C2)C4=C(C=C([*])S4)C=C3	33.88	10.71
	[*]C1=CC2=C(S1)C=CC3=C2C=CC4=C3C=C([*])S4	34.55	10.92

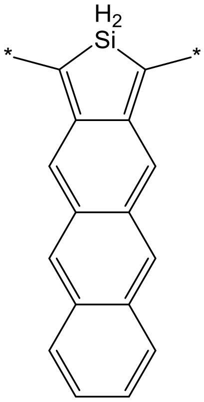
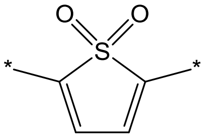
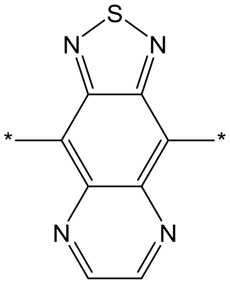
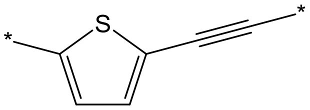
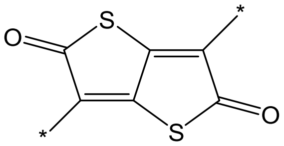
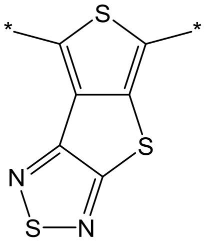
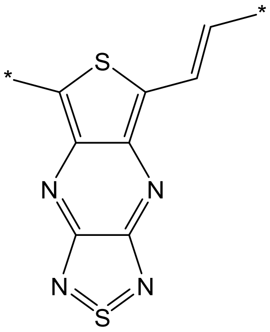
	CN1C(C2=CC([*])=C(C3=O)C4=C2C(C1=O)=C([*])C=C4C(N3C)=O)=O	32.54	13.28
	[*]C1=CC=C([*])N1	12.62	6.31
	[*]C1=CC=C(/C=C/[*])N1	11.48	4.69
	[*]C1=C(C=CC=C2)C2=C([*])N1	-2.25	-1.12
	[*]C1=C(C=C(C=CC=C2)C2=C3)C3=C([*])N1	-8.70	-4.35
	[*]C1=C(C=C(C=C(C=CC=C2)C2=C3)C3=C4)C4=C([*])N1	-11.80	-5.90
	[*]C1=CC=C([*])O1	11.42	5.71
	[*]C1=CC=C(/C=C/[*])O1	10.15	4.15

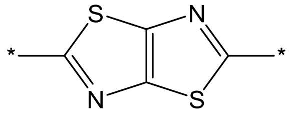
	[*]C1=C(C=CC=C2)C2=C([*])O1	-6.12	-3.06
	[*]C1=C(C=C(C=CC=C2)C2=C3)C3=C([*])O1	-13.77	-6.89
	[*]C1=C(C=C(C=C(C=CC=C2)C2=C3)C3=C4)C4=C([*])O1	-15.85	-7.93
	[*]C1=C([*])N=CN1	15.51	10.97
	[*]C1=C([*])N=CS1	15.10	10.68
	[*]C1=C(C(SC2=O)=O)C2=C([*])S1	18.56	9.28
	[*]C1=C(C(SC2=O)=O)C2=C([*])O1	18.68	9.34

	[*]C1=C(C(SC2=O)=O)C2=C([*])N1	22.82	11.41
	[*]C1=C(C(OC2=O)=O)C2=C([*])S1	17.26	8.63
	[*]C1=C(C(OC2=O)=O)C2=C([*])N1	21.40	10.70
	[*]C1=C(C(OC2=O)=O)C2=C([*])O1	17.48	8.74
	[*]C1=C(C(NC2=O)=O)C2=C([*])S1	17.64	8.82
	[*]C1=C(C(NC2=O)=O)C2=C([*])N1	20.93	10.46
	[*]C1=C(C(NC2=O)=O)C2=C([*])O1	17.61	8.80
	[*]C#CC1=CC=C([*])C=C1	30.96	12.64
	[*]C1=CC=C([*])S1	12.19	6.09

	[*]C1=CC=C(/C=C/[*])S1	10.59	5.29
	[*]C1=C(C=CC=C2)C2=C([*])S1	-3.25	-1.63
	[*]C1=C(C=CC=C2)C2=C(/C=C/[*])S1	-4.18	-2.09
	[*]C1=C(C=C(C=CC=C2)C2=C3)C3=C([*])S1	-9.96	-4.98
	[*]C1=C(C=C(C=CC=C2)C2=C3)C3=C(/C=C/[*])S1	-10.82	-5.41
	[*]C1=C(C=C(C=C(C=CC=C2)C2=C3)C3=C4)C4=C([*])S1	-12.06	-6.03
	[*]C1=CC=C([*])[Se]1	9.75	4.87
	[*]C1=CC=C(/C=C/[*])[Se]1	8.44	3.44

	[*]C1=C(C=CC=C2)C2=C([*])[Se]1	-6.09	-3.05
	[*]C1=C(C=C(C=CC=C2)C2=C3)C3=C([*])[Se]1	-13.11	-6.56
	[*]C1=C(C=C(C=C(C=CC=C2)C2=C3)C3=C4)C4=C([*])[Se]1	-14.65	-7.33
	[*]C1=CC=C([*])[SiH2]1	-0.79	-0.40
	[*]C1=C(C=CC=C2)C2=C([*])[SiH2]1	-22.46	-11.23
	[*]C1=C(C=C(C=CC=C2)C2=C3)C3=C([*])[SiH2]1	-26.74	-13.37

	[*]C1=C(C=C(C=C(C=CC=C2)C2=C3)C3=C4)C4=C([*])[SiH2]1	-24.78	-12.39
	[*]C1=CC=C([*])S1(=O)=O	4.47	2.23
	[*]C1=C(N=CC=N2)C2=C([*])C3=NSN=C31	-1.59	-0.79
	[*]C1=CC=C(C#C[*])S1	20.05	8.19
	O=C1C([*])=C(S2)C(S1)=C([*])C2=O	13.15	6.58
	[*]C1=C(C2=NSN=C2S3)C3=C([*])S1	10.82	5.41
	[*]C1=C(N=C(N=S=N2)C2=N3)C3=C(/C=C/[*])S1	-13.64	-5.57

	[*]C1=NC2=C(S1)N=C([*])S2	18.51	7.55

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