Supporting Information

Novel perylene-based organic dyes for Electro-fluidic display

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Contents

Figure S1. IR spectrum of P-Br (KBr) ................................................................. 2
Figure S2. 1H NMR (400 MHz) spectrum of P-Br in CDCl3 .................................... 3
Figure S3. 13C NMR (400 MHz) spectrum of P-Br in CDCl3 ................................. 4
Figure S4. MS (MALDI-TOF) of P-Br ................................................................. 5
Figure S5. IR spectrum of Y-1 (KBr) ................................................................. 6
Figure S6. 1H NMR (400 MHz) spectrum of Y-1 in CDCl3 ................................. 7
Figure S7. 13C NMR (400 MHz) spectrum of Y-1 in CDCl3 ................................. 8
Figure S8. MS (MALDI-TOF) of Y-1 ................................................................. 9
Figure S9. IR spectrum of O-1 (KBr) ................................................................. 10
Figure S10. 1H NMR (400 MHz) spectrum of O-1 in CDCl3 ............................... 11
Figure S11. 13C NMR (400 MHz) spectrum of O-1 in CDCl3 ............................... 12
Figure S12. MS (MALDI-TOF) of O-1 ............................................................... 13
Figure S13. IR spectrum of R-1 (KBr) ............................................................... 14
Figure S14. 1H NMR (400 MHz) spectrum of R-1 in CDCl3 ............................... 15
Figure S15. 13C NMR (400 MHz) spectrum of R-1 in CDCl3 ............................... 16
Figure S16. MS (MALDI-TOF) of R-1 ............................................................... 17
Figure S17. IR spectrum of M-1 (KBr) ............................................................... 18
Figure S18. 1H NMR (400 MHz) spectrum of M-1 in CDCl3 ............................... 19
Figure S19. 13C NMR (400 MHz) spectrum of M-1 in CDCl3 ............................... 20
Figure S20. MS (MALDI-TOF) of M-1 ............................................................... 21
Figure S21. IR spectrum of C-1 (KBr) ............................................................... 22
Figure S22. 1H NMR (400 MHz) spectrum of C-1 in CDCl3 ............................... 23
Figure S23. 13C NMR (400 MHz) spectrum of C-1 in CDCl3 ............................... 24
Figure S24. MS (MALDI-TOF) of C-1 ............................................................... 25
Table 1. The Element analysis of six formulated molecules ................................... 25
Figure S25. Curves of molar extinction coefficient versus concentration for O-1 .......... 26
Figure S26. Curves of molar extinction coefficient versus concentration for M-1 ......... 27
Figure S27. Curves of molar extinction coefficient versus concentration for R-1 ......... 27
Figure S28. Curves of molar extinction coefficient versus concentration for C-1 .......... 28
Figure S29. Minimized structures of compounds M-1. .......................................... 30
1. Structure characterization original spectra

1.1. IR spectrum of P-Br (KBr)

Fourier transform infrared spectroscopy (FT-IR) was recorded on a PerkinElmer Spectrum One FT-IR Spectrometer in the range of 4000−400 cm$^{-1}$. Samples of Perylene-derived dyes were prepared by mixing into a thin film on a KBr plate. The peak at 2922 cm$^{-1}$ and 2860 cm$^{-1}$ for substituted Perylene dimide is assigned as the symmetric NC−H stretching vibration of methyl group linked to the imide nitrogen. The peaks at 3093 and 3118 cm$^{-1}$ are the symmetric and asymmetric stretching vibration of C-H at position 1, 2, 5, 6, 7, 8, 11 and 12 of perylene ring. The symmetric C=O stretching vibrations of PDI-Br appeared at 1680 cm$^{-1}$, respectively. The introduction of side atoms at 1, 7 positions of perylene ring do not affect these two vibrations and the peaks keep unchanged in the spectra of other compounds. The peak at 1581 cm$^{-1}$ in the spectrum of PDI-Br corresponds to the wag vibration of C-H on the perylene ring, which are also unaffected by the side groups as revealed by the spectra of other compounds. In the range of 1570-1330 cm$^{-1}$, a group of small peaks were found in the spectrum of PDI-Br, which are assigned to the inplane C-H wag and/or C=C stretching of the perylene ring. The peaks in the region of 1000-1330 cm$^{-1}$ are assigned to the vibration of deformation of perylene ring and the imide ring.
1.2. $^1$H NMR (400 MHz) spectrum of P-Br in CDCl$_3$

As the structure of the perylene dyes is shown in the Figure S1, the different peaks belong to the protons. The “H1” and “H2” protons appear as one singlet and one doublet between 9.432 and 8.8 ppm. The “H3” protons appear as a doublet between 8.642 and 8.625 ppm. “H4” for the methine protons present in amino group. The multiple peak at 3.8 ppm presents “H5”. The other peaks such as “H6-7” and “H8-9” represent the alkyl protons. The ratio of different protons is 1: 1: 1: 2: 1: 32:6, which is just consistent with the real value of different proton. Because the solvent impurity n-pentane is not removed thoroughly, there is still excess peaks appearing 2.25-1.5ppm.
1.3. $^{13}$C NMR (400 MHz) spectrum of P-Br in CDCl$_3$

As the $^{13}$C NMR (400 MHz) spectrum of P-Br in CDCl$_3$ is shown in the Figure S3, C1-11 represent the aromatic carbons, which appears between 115 and 165 ppm. The “C1” carbon appears as a doublet between 160 and 165 ppm. The “C2” and “C3” protons appear as one singlet and one doublet between 130 and 135 ppm. “C4” carbon appears in 128 ppm. Other signals C5, C7, C8, C11
attributable to the core carbon can be identified as 122.5, 123.1, 124.3, and 121.1; Analyzing about the ratio of the different carbon number, the ratio is 2:1:2:1:1:1:1. For symmetric structure the number of scales by 2 is the actual number of each carbon atom. The chemical shift of a carbon atom is 13-46 ppm which is the location of fatty carbon. The chemical shift of the “C12” carbons for alkyl-substituted BPTIs appear slightly to 45.3 ppm.”C13” shift at 36.8 ppm.”C14” “C15” appear as 31.5-32 ppm. The long alkyl carbon position show between 29 and 30 ppm. “C16” and “C17” appears at 26.9 ppm. The other two peaks represent “C28-C29” and “C30-C31”. The ratio of these carbons shows 1:1:2:10:2:2:2.

1.4. MS (MALDI-TOF) of R-1

![Graph showing MS (MALDI-TOF) of R-1](image)

The molecular ion obtained after Y-1 loses a proton, and the mass-to-charge ratio measured according to MALDI-TOF is 1108.52, Calcd for C62H92O4 (m/z) 1108.52.
1.5. IR spectrum of Y-1(KBr)

Figure S4. IR spectrum of Y-1 (KBr)

The simulated IR spectra of these compounds are shown in Figure S4. The peaks at 2850 and 2920 cm⁻¹ are the symmetric and asymmetric stretching vibration of C – H at position 1, 2, 5, 6, 7, 8, 11 and 12 of perylene ring. The asymmetric and symmetric C=O stretching vibrations of Perylene dyes appeared at 1680 cm⁻¹. The small peaks at 1493 cm⁻¹ for O-C with obviously increased intensity. The peaks were shifted to 1373 cm⁻¹ and 1430 cm⁻¹ in the spectrum of -CH-. The peaks in the region of 1000-1420 cm⁻¹ are assigned to the vibration of deformation of perylene ring.
1.6. $^1$H NMR (400 MHz) spectrum of Y-1 in CDCl$_3$

![Figure S5. $^1$H NMR (400 MHz) spectrum of Y-1 in CDCl$_3$.]

As the structure of the perylene dyes is shown in the Figure S5, the different peaks belong to the protons. The “H1” and “H2” protons appear as two doublets between 7.5 and 7.6 ppm. The “H3” protons appear as one singlet between 8.142 and 8.225 ppm. “H4” and “H5” protons appear as two doublets at 8.872 and 8.955 ppm. “H6” for the methine protons present in amino group at 4.3 ppm. The peaks between 0.5 and 2.0 ppm present “H7-13” represent the alkyl protons. “H12-13” show at 0.5 ppm for the terminal methyl proton. The ratio of different protons is 1:1:1:1:2:1:4:24:4:6, which is just consistent with the real value of different proton. Because the solvent impurity n-pentane is not removed thoroughly, there is still excess peaks appearing 2.25-1.5 ppm.
1.7. $^{13}$C NMR (400 MHz) spectrum of Y-1 in CDCl$_3$

![Diagram of molecular structure](image)

(a). $^{13}$C NMR (400 MHz) full spectrum of Y-1 in CDCl$_3$

(b). $^{13}$C NMR (400 MHz) part spectrum(120-188ppm) of Y-1 in CDCl$_3$

(c). $^{13}$C NMR (400 MHz) part spectrum(8-88ppm) of Y-1 in CDCl$_3$

Figure S6. $^{13}$C NMR (400 MHz) spectrum of Y-1 in CDCl$_3$.

As the $^{13}$C NMR (400 MHz) spectrum of Y-1 in CDCl$_3$ is shown in the FigureS6, C1-11 represent the aromatic carbons, which appears between 120 and 168ppm. The “C1” carbon appears as a doublet between 167.8ppm. The “C3” and “C4” protons appear as one singlet and one doublet between 130 and 135ppm. “C4” carbon appears in 128 ppm. Other signals C5,C7,C8,C11 attributable to the core carbon can be identified as 133.5,127.1, 122.3, and 131.1; “C6” carbon appears in 126.8 ppm. “C9” carbon appears in 121.5 ppm. “C10” carbon appears in 119.8 ppm. The ratio of the different carbon number is 1:1:1:1:1:1:1:1:1:1:1. For symmetric structure the of perylene dyes, multiplying the number of scales by 2 is the actual number of each carbon atom. The chemical shift of a carbon atom is 8-70 ppm which is the location of fatty carbon. The chemical shift of the “C12” carbons for alkyl-substituted BPTIs appear slightly to 45.3ppm.”C13” shift at 36.8ppm. ”C14” “C15” appear as 31.5-32ppm. The long alkyl carbon position “C18-27” show between 28 and 30ppm.”C16”and “C17” appears at 26.9ppm. The other two peaks represent “C28-C29” and “C30-C31”. The ratio of these carbons shows 1:1:1:2:2:6:2:2:6:2.
1.8. MS (MALDI-TOF) of Y-1

The molecular ion obtained after Y-1 loses a proton, and the mass-to-charge ratio measured according to MALDI-TOF is 900.70, Calcd for C62H92O4 (m/z) 900.70.
1.9. IR spectrum of O-1(KBr)

Figure S8. IR spectrum of O-1 (KBr).

Fourier transform infrared spectroscopy (FT-IR) was recorded on a PerkinElmer Spectrum One FT-IR Spectrometer in the range of 4000–400 cm⁻¹. Samples of Perylene-derived dyes were prepared by mixing into a thin film on a KBr plate. The peak at 2922 cm⁻¹ and 2860 cm⁻¹ for substituted PDI is assigned as the symmetric NC–H stretching vibration of methyl group linked to the imide nitrogen. The peaks at 3093 and 3118 cm⁻¹ are the symmetric and asymmetric stretching vibration of C-H at position 1, 2, 5, 6, 7, 8, 11 and 12 of perylene ring. The symmetric C=O stretching vibrations of PDI-Br appeared at 1680 cm⁻¹, respectively. The introduction of side atoms at 1,7 positions of perylene ring do not affect these two vibrations and the peaks keep unchanged in the spectra of other compounds. In the range of 1570-1330 cm⁻¹, a group of small peaks were found in the spectrum of PDI, which are assigned to the inplane C-H wag and/or C=C stretching of the perylene ring. The peaks in the region of 1000-1330 cm⁻¹ are assigned to the vibration of deformation of perylene ring and the imide ring.

1.10. ¹H NMR (400 MHz) spectrum of O-1 in CDCl₃
As the structure of the perylene dyes is shown in the Figure S9, the different peaks belong to the protons. The “H1” and “H2” protons appear as one singlet and one multiplet between 8.5 and 9.0 ppm. “H3” for the methine protons present in amino group at 4.23 ppm. The peaks between 0 and 2.0 ppm present “H4-7” represent the alkyl protons. “H7-8” show at 0.5 ppm for the terminal methyl proton. The ratio of different protons is 2: 2: 2: 1: 32: 6, which is just consistent with the real value of different proton. Because the solvent impurity n-pentane is not removed thoroughly, there is still excess peaks appearing 1.5-2.0 ppm.
1.11. ¹³C NMR (400 MHz) spectrum of O-1 in CDCl₃

(a). ¹³C NMR (400 MHz) full spectrum of O-1 in CDCl₃.

(b). ¹³C NMR (400 MHz) part spectrum (122-166ppm) of O-1 in CDCl₃.

(c). ¹³C NMR (400 MHz) part spectrum (2-48ppm) of O-1 in CDCl₃.

Figure S10. ¹³C NMR (400 MHz) spectrum of O-1 in CDCl₃.

As the ¹³C NMR (400 MHz) spectrum of P-Br in CDCl₃ is shown in the FigureS10, C1-7 represent the aromatic carbons, which appears between 122 and 165ppm. The “C1” carbon appears as a singlet at 163.7ppm. The “C2” protons appear as one singlet and one doublet between 131.5 ppm. “C3-4” carbon appears between 121 and 123 ppm. Other signals “C5”, “C6”, ”C7” attributable to the core carbon can be identified as 134.5,129.3 and 126.5; Analysing about the ratio of the different carbon number, the ratio is 2:2:1:1:8. For symmetric structure the of perylene dyes, multiplying the number of scales by 2 is the actual number of each carbon atom. The chemical shift of a carbon atom is 3-46 ppm which is the location of fatty carbon. The chemical shift of the “C8” carbons for
alkyl-substituted BPTIs appear slightly to 44.8 ppm. "C9" shift at 36.8 ppm. The long alkyl carbon position “C18-27” show between 29 and 30 ppm. C16” and “C17” appear at 26.9 ppm. The other two peaks represent “C10-C11” and “C30-C31”. The ratio of these carbons shows 1:1:6:4:2:2:2:2.

1.12. MS (MALDI-TOF) of O-1

![MS (MALDI-TOF) of O-1](image)

The molecular ion obtained after O-1 loses a proton, and the mass-to-charge ratio measured according to MALDI-TOF is 950.70, Calcd for C64H90N2O4 (m/z) 950.7029.
1.13. IR spectrum of R-1(KBr)

When methyl containing groups (CH$_3$O–) are introduced to the 1, 7 positions of perylene dye, the peak at 2970 cm$^{-1}$, corresponding to the symmetric stretching of C–H of the methyl group attached at imide nitrogen, are intensified by the side groups following the order of CH$_3$O–, while the peaks at 3093 and 3118 cm$^{-1}$ are weakened significantly or even more completely disappeared. The newly appeared peaks at 2922 cm$^{-1}$ for O-C and 2860 cm$^{-1}$ for N-a are assigned to the symmetric XC–H (X = O) stretching of the introduced methoxy and methylamino groups respectively. The peaks at 2993 and 3044 cm$^{-1}$ in the IR spectra of O-C, which do not shown in the spectra of other N-compounds, are assigned to the symmetric and asymmetric OC-H stretching vibration of methoxy groups. Same vibration of methylamino groups in N-a appeared at 2979 and 3448 cm$^{-1}$. Four peaks at 2926, 2952 2993 and 3044 cm$^{-1}$ were assigned to the OC-H stretching vibrations. Six peaks at 2905, 2925, 2990, 2979, 3042 and 3448 cm$^{-1}$ were found in the IR spectra of N-a, which are assigned similarly to the symmetrical or asymmetrical stretching vibration of NC-H of methylamino groups. For compounds O-C, the peaks corresponding to the stretching vibration of C-H on the perylene ring appeared at 2970 and 3028 cm$^{-1}$. A large new peak near 3088 cm$^{-1}$ was assigned to the C-H stretching vibration of benzene in phenoxy groups. The introduction of side groups at 1, 7 positions of perylene ring do not affect these two vibrations and the peaks keep unchanged in the spectra of other compounds. The peak at 1581 cm$^{-1}$ in the spectrum corresponds to the wag vibration of C–H on the perylene ring, which are also unaffected by the side groups as revealed by the spectra of other compounds. In the range of 1570-1450 cm$^{-1}$, a group of small peaks were found in the spectrum of PDI-0, which are assigned to the inplane C-H wag and/or C=C stretching of the perylene
ring. These peaks were found to be affected by the side groups. The small shoulder at 1493 cm\(^{-1}\) in the spectrum shifts to a lower wave number when side groups are introduced. The same peaks were shifted to 1485 and 1455 cm\(^{-1}\) in the spectrum of N-a. The results suggest that the substitution of side groups at bay positions affect the vibrations of C=C stretching in the perylene ring. The peaks in the region of 1000-1420 cm\(^{-1}\) are assigned to the vibration of deformation of perylene ring and the imide ring. The introduction of side groups brings large changes on both the position and intensity of the peaks in this region. Because the symmetry of the molecule were reduced by the introduction of side groups at 1, 7 positions, which brings more vibration models for the molecules, and thus results in more peaks in this region.

1.14. \(^1\)H NMR (400 MHz) spectrum of R-1 in CDCl\(_3\)

As the structure of the perylene dyes is shown in the Figure S13, the different peaks belong to the protons. The “H1” and “H2” protons appear as one singlet and one multiplet between 8.25 and 8.56 ppm. The “H3” protons appear as a triplet at 9.57 ppm. “H5” and “H6” protons appear as two doublets at 7.35 and 7.0ppm. “H4” for the methine protons present in amino group at 4.0 ppm. The “H9” protons appear as a triplet between 3.67 ppm. The peaks between 0 and 2.0ppm present the alkyl protons. “H16-17” show at 0.5ppm for the terminal methyl proton. The ratio of different protons is 1: 1: 1: 2: 2: 2: 1: 2: 4: 6: 4: 24: 4: 6, which is just consistent with the real value of different proton. Because the solvent impurity n-pentane is not removed thoroughly, there is still excess peaks appearing 2.25-1.5ppm.

1.15. \(^{13}\)C NMR (400 MHz) spectrum of R-1 in CDCl\(_3\)
Figure S14. $^{13}$C NMR (400 MHz) spectrum of R-1 in CDCl₃

As the $^{13}$C NMR (400 MHz) spectrum of P-Br in CDCl₃ is shown in the FigureS14, C1-13 represent the aromatic carbons, which appears between 118 and 165ppm. The “C1” carbon appears as a singlet at 163.7ppm. The “C2” protons appear as one singlet and one doublet between 130.5 ppm. “C3-4,6” carbon appears between 128 ppm. Other signals C7, C8, C9, C10, C11, C12, C13 attributable to the core carbon can be identified as 153.5,122.3, 133.3,125.2, 128.9 and 155.5; Analysing about the ratio of the different carbon number, the ratio is 2:1:1:1:1:1:1:2:1:2:1. For symmetric structure the of perylene dyes, multiplying the number of scales by 2 is the actual number of each carbon atom.

(a).$^{13}$C NMR (400 MHz) full spectrum of R-1 in CDCl₃

(b).$^{13}$C NMR (400 MHz) part spectrum(118-166ppm) of R-1 in CDCl₃

(c).$^{13}$C NMR (400 MHz) part spectrum(10-58ppm) of R-1 in CDCl₃
The chemical shift of a carbon atom is 10-58 ppm which is the location of fatty carbon. The chemical shift of the “C37” carbons for alkyl-substituted BPTIs appear slightly to 56.8 ppm. “C16” shift at 38.5 ppm. The long alkyl carbon position “C18-33” show between 28 and 30 ppm. “C21-22” appears at 26.7 ppm. The other two peaks represent “C10-C11” and “C30-C31”. “C17” and “C38” appears at 32.1 ppm. “C34-35” appears at 14.5 ppm. “C39” appears at 22.9 ppm. The ratio of these carbons shows 1:1:1:1:15:2:2:2.

1.16. MS (MALDI-TOF) of R-1

Figure S15. MS (MALDI-TOF) of R-1

The molecular ion obtained after R-1 loses a proton, and the mass-to-charge ratio measured according to MALDI-TOF is 1360.00, Calcd for C92H120N2O6 (m/z) 1360.00.
1.17. IR spectrum of M-1 (KBr)

When methyl containing groups (CH3O⁻) are introduced to the 1, 7 positions of PDI, the peak at 2970 cm⁻¹, corresponding to the symmetric stretching of C–H of the methyl group attached at imide nitrogen, are intensified by the side groups following the order of CH3O⁻, while the peaks at 3093 and 3118 cm⁻¹ are weakened significantly or even more completely disappeared. The newly appeared peaks at 2926 cm⁻¹ for O-a and 2902 cm⁻¹ for N-a are assigned to the symmetric XC–H (X = O) stretching of the introduced methoxy and methylamino groups respectively. The peaks at 2993 and 3044 cm⁻¹ in the IR spectra of O-a, which do not show in the spectra of other compounds, are assigned to the symmetric and asymmetric OC–H stretching vibration of methoxy groups. Same vibration of methylamino groups in N-a appeared at 2979 and 3448 cm⁻¹. Four peaks at 2926, 2952 2993 and 3044 cm⁻¹ were assigned to the OC-H stretching vibrations stretching vibration of NC-H of methylamino groups. For compounds O-b, the peaks corresponding to the stretching vibration of C–H on the perylene ring appeared at 2970 and 3028 cm⁻¹. A large new peak near 3088 cm⁻¹ was assigned to the C-H stretching vibration of benzene in alkoxy groups. The asymmetric and symmetric C=O stretching vibrations of PDI-0 appeared at 1706 and 1674 cm⁻¹, respectively. The introduction of side groups at 1, 7 positions of perylene ring do not affect these two vibrations and the peaks keep unchanged in the spectra of other compounds. The peak at 1581 cm⁻¹ in the spectrum of PDI corresponds to the wag vibration of C-H on the perylene ring, which are also unaffected by the side groups as revealed by the spectra of other compounds. In the range of 1570-1450 cm⁻¹, a group of small peaks were found in the spectrum of PDI, which are assigned to the inplane C-H wag
and/or C=C stretching of the perylene ring. These peaks were found to be affected by the side groups. The small shoulder at 1567 cm$^{-1}$ in the spectrum of PDI-0 shifts to a lower wave number when side groups are introduced. The small peaks at 1463 cm$^{-1}$ for O-a with obviously increased intensity. The same peaks were shifted to 1485 and 1455 cm$^{-1}$ in the spectrum of N-C. The results suggest that the substitution of side groups at bay positions affect the vibrations of C=C stretching in the perylene ring. The peaks in the region of 1000-1420 cm$^{-1}$ are assigned to the vibration of deformation of perylene ring and the imide ring. The introduction of side groups brings large changes on both the position and intensity of the peaks in this region. Because the symmetry of the molecule were reduced by the introduction of side groups at 1, 7 positions, which brings more vibration models for the molecules, and thus results in more peaks in this region. It is worth noting that the IR spectra of O-C comprise most of the feather peaks of O-C.

1.18. $^1$H NMR (400 MHz) spectrum of M-1 in CDCl$_3$

As the structure of the perylene dyes is shown in the FigureS17, the different peaks belong to the protons. The “H1” and “H2” protons appear as two singlet between 9.432 and 8.8 ppm. The “H3” protons appear as a singlet at 9.625 ppm. “H4” for the methine protons as a singlet present in amino group at 4.125ppm. The multiple peak at 4.282 ppm presents “H6”. The other peaks such as “H5” and “H8-15” represent the alkyl protons between 1.250 to 1.500ppm. “H16-17” “H18” and “H19” show at 0.785ppm,1.285ppm, and 1.000ppm for the all terminal methyl proton. The ratio of different protons is 1:1:2:2:2:40:3:3:6, which is just consistent with the real value of different proton.Because the solvent impurity n-pentane is not removed thoroughly, there is still excess peaks appearing 2.25-1.5ppm.

1.19. $^{13}$C NMR (400 MHz) spectrum of M-1 in CDCl$_3$
As the $^{13}$C NMR (400 MHz) spectrum of M-1 in CDCl$_3$ is shown in the Figure S18, C1-13 represent the aromatic carbons, which appears between 114 and 166 ppm. The “C1” carbon appears as a singlet at 163.7 ppm. The “C4” protons appear as one singlet at 156.2 ppm. “C5” carbons appears at 133.8 ppm. Other signals C2, C3, C6, C7-8, C9, C10, C11 attributable to the core carbon can be identified as 128.5, 121.3, 128.8, 117.4, 121.2, 123.6 and 128.9 ppm. Analysing about the ratio of the different carbon number, the ratio is 2:1:1:2:1:1:1:2:2. For symmetric structure the of perylene dyes, multiplying the number of scales by 2 is the actual number of each carbon atom. The chemical shift of a carbon
atom is 5-75 ppm which is the location of fatty carbon. The chemical shift of the “C32” carbons for alkyl-substituted BPTIs appear slightly to 72.8 ppm. “C12” shift at 45.5 ppm. The long alkyl carbon position “C19-27” show between 28 and 30 ppm. “C12” appears at 39.7 ppm. “C13” and “C14-15” appears at 37.1 ppm and 32.3 ppm. “C16-17” appears at 28.5 ppm. “C18” appears at 31.9 ppm. “H30-31” and “H39” show at 13.8 ppm for the all terminal methyl carbon. The ratio of these carbons shows 1:1:1:2:2:2:2:3.

1.20. MS (MALDI-TOF) of M-1

The molecular ion obtained after M-1 loses a proton, and the mass-to-charge ratio measured according to MALDI-TOF is 1206.93. Calcd for C80H122N2O6 (m/z) 1206.93.

1.21. IR spectrum of C-1(KBr)
When methyl containing groups (CH3N-) are introduced to the 1,7 positions of PDI, the peak at 2922 cm\(^{-1}\), corresponding to the symmetric stretching of C-H of the methyl group attached at imide nitrogen, are intensified by the side groups following the order of CH3N-, while the peaks at 3093 and 3118 cm\(^{-1}\) are weakened significantly or even more completely disappeared. The newly appeared peaks at 2922 cm\(^{-1}\) N-C are assigned to the symmetric XC=CH (X= N) stretching of the introduced methoxy and methylamino groups respectively. Same vibration of methylamino groups in N-C appeared at 2979 and 3448 cm\(^{-1}\). Four peaks at 2860, 2922, 3011 and 3093 cm\(^{-1}\) were found in the IR spectra of N-C, which are assigned similarly to the symmetrical or asymmetrical stretching vibration of NC-H of methylamino groups. A large new peak near 3088 cm\(^{-1}\) was assigned to the C-H stretching vibration of benzene in phenoxy groups. The asymmetric and symmetric C=O stretching vibrations of perylene appeared at 1680 cm\(^{-1}\), respectively. The introduction of side groups at 1, 7 positions of perylene ring do not affect these two vibrations and the peaks keep unchanged in the spectra of other compounds. The peak at 1581 cm\(^{-1}\) in the spectrum of PDI corresponds to the wag vibration of C-H on the perylene ring, which are also unaffected by the side groups as revealed by the spectra of other compounds. In the peak of 1493 cm\(^{-1}\), a group of small peaks were found in the spectrum of PDI, which are assigned to the inplane C-H wag and/or C=C stretching of the perylene ring. These peaks were found to be affected by the side groups. The small shoulder at 1567 cm\(^{-1}\) in the spectrum of PDI shifts to a lower wave number when side groups are introduced. The small peaks at 1468 cm\(^{-1}\) for PDI shifted to 1493 for N-C with obviously increased intensity. The same peaks were shifted to 1485 and 1455 cm\(^{-1}\) in the spectrum of N-C. The results suggest that the substitution of side groups at bay positions affect the vibrations of C=C stretching in the perylene ring. The peaks in the region of 1000-1420 cm\(^{-1}\) are assigned to the vibration of deformation of perylene ring and the imide ring. The introduction of side groups brings large changes on both the position and intensity of the peaks in this region. Because the symmetry of the
molecule were reduced by the introduction of side groups at 1, 7 positions, which brings more vibration models for the molecules, and thus results in more peaks in this region. It is worth noting that the IR spectra of ON-C comprise the most feather peaks of N-C and O-C.

1.22. $^1$H NMR (400 MHz) spectrum of C-1 in CDCl$_3$

![Figure S21. $^1$H NMR (400 MHz) spectrum of C-1 in CDCl$_3$](image)

As the structure of the perylene dyes is shown in the FigureS21, the different peaks belong to the protons. The “H1” and “H2” protons appear as one singlet and one doublet between 8.25 and 8.5 ppm. The “H3” protons appear as a singlet 9.635 ppm. “H5” protons appear as two doublets at 3.5 ppm. “H4” for the methine protons present in amino group at 4.2 ppm. “H6” protons appear as two triplets at 2.75 ppm. The peaks between 0 and 2.0ppm present “H7-9” represent the alkyl protons. “H11-14” and “H9” show at 0.5ppm for the terminal methyl proton. The ratio of different protons is 1: 1: 1: 2: 2: 4:34: 6, which is just consistent with the real value of different proton. Because the solvent impurity n-pentane is not removed thoroughly, there is still excess peaks appearing 2.25-1.5ppm.

1.23. $^{13}$C NMR (400 MHz) spectrum of C-1 in CDCl$_3$
As the $^{13}$C NMR (400 MHz) spectrum of P-Br in CDCl$_3$ is shown in the Figure S22, C1-10 represent the aromatic carbons, which appears between 116 and 165 ppm. The “C1” carbon appears as a singlet at 164.7 ppm. The “C8” protons appear as one singlet at 163.5 ppm. “C6” carbon appears between 138 ppm. Other signals C2,C3,C4,C5,C7,C9 and C10 attributable to the core carbon can be identified as 136.5, 131, 134.5, 130.2, 118.5, 121.1 and 128.2; Analysing about the ratio of the different carbon number, the ratio is 2:1:1:1:1:2:1:1. For symmetric structure the of perylene dyes, multiplying the number of scales by 2 is the actual number of each carbon atom. The chemical shift of a carbon atom is 14-54 ppm which is the location of fatty carbon. The chemical shift of the “C11” carbons for alkyl-substituted BPTIs appear slightly to 53.2 ppm.”C13” shift at 44.8 ppm”. The long alkyl carbon position “C16-23” show between 32 and 33 ppm”. C14-15” appears at 36.8 ppm. “C12” shift at 32.0 ppm. The other two peaks represent “C28-29” and “C24-25” between 26 to 28 ppm. C26-27” appears at 23.8 ppm.”H30-31” show at 14.2 ppm for the all terminal methyl carbon. The ratio of these carbons shows 2:1:2:1:6:2:2:2:2:12.

1.24. MS (MALDI-TOF) of C-1
The molecular ion obtained after C-1 loses a proton, and the mass-to-charge ratio measured according to MALDI-TOF is 1116.84, Calcd for C74H108N4O4 (m/z) 1116.84.

**Element analysis:**

Table 1. The Element analysis of six formulated molecules.

<table>
<thead>
<tr>
<th>Dyes</th>
<th>Found N [%]</th>
<th>Found C [%]</th>
<th>Found H [%]</th>
<th>Found O [%]</th>
<th>Calcd N [%]</th>
<th>Calcd C [%]</th>
<th>Calcd H [%]</th>
<th>Calcd O [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>P-Br</td>
<td>2.45</td>
<td>69.68</td>
<td>8.04</td>
<td></td>
<td>2.52</td>
<td>69.3</td>
<td>8.01</td>
<td></td>
</tr>
<tr>
<td>Y-1</td>
<td>0</td>
<td>82.55</td>
<td>10.09</td>
<td>7.36</td>
<td>0</td>
<td>82.61</td>
<td>10.29</td>
<td>7.1</td>
</tr>
<tr>
<td>O-1</td>
<td>2.93</td>
<td>80.69</td>
<td>9.449</td>
<td>6.931</td>
<td>2.94</td>
<td>80.79</td>
<td>9.54</td>
<td>6.73</td>
</tr>
<tr>
<td>R-1</td>
<td>2.43</td>
<td>79.99</td>
<td>9.50</td>
<td>8.08</td>
<td>2.39</td>
<td>80.54</td>
<td>9.8</td>
<td>7.27</td>
</tr>
<tr>
<td>M-1</td>
<td>2.31</td>
<td>79.85</td>
<td>9.73</td>
<td>8.11</td>
<td>2.32</td>
<td>79.55</td>
<td>10.18</td>
<td>7.95</td>
</tr>
<tr>
<td>C-1</td>
<td>4.69</td>
<td>79.34</td>
<td>9.72</td>
<td>6.25</td>
<td>4.69</td>
<td>79.52</td>
<td>9.74</td>
<td>6.05</td>
</tr>
</tbody>
</table>

According to the elemental analysis data, the percentage of elements of the five synthetic molecules is consistent with the theoretical value. Thus, it is demonstrated the consistency of the experimental synthetic molecules with the designed molecular structure.

**2. Solubility test**

Preparation of saturated solution of formulated dyes(O-1,R-1,M-1,C-1) (solvent is n-decane): To a reactor was added a mixture of formulated dyes and n-decane, dissolve by ultrasonic stirring 1h, and rest for 2 days. The mixture was centrifuged (10000r/min, 10min) to remove excess insoluble
dye. A certain amount of supernatant was measured by a Pipette and to be diluted to a certain multiple. The absorbance was measured by UV-vis, the diluted concentration $c$ was calculated according to the formula $A = \varepsilon \cdot d \cdot c$, ($\varepsilon$ is obtained by absorption experiment) and finally the mass fraction wt% of the saturated solution before dilution were obtained.

2.1. Solubility test of O-1

To a reactor was added a mixture of 0.15g of O-1 and 0.5mL n-decane, dissolve by ultrasonic stirring 1h, and rest for 2 days. The mixture was centrifuged (10000r/min, 10min)) to remove excess insoluble dye. 50μL of supernatant was measured by a Pipette and to be diluted to 25mL of solvent. The absorbance was measured by UV-vis ($A = 2.26$), the diluted concentration $c$ was calculated to be $4.346 \times 10^{-5}$mol/L according to the formula $A = \varepsilon \cdot d \cdot c$ ($\varepsilon(A = 2.456) = 52000$) and finally the mass fraction wt% of the saturated solution before dilution were obtained to be 2.82%

2.2. Solubility test of M-1
Figure S25. Curves of molar extinction coefficient versus concentration for M-1.

To a reactor was added a mixture of 0.19g of M-1 and 0.5mL n-decane, dissolve by ultrasonic stirring 1h, and rest for 2 days. The mixture was centrifuged (10000r/min, 10min)) to remove excess insoluble dye. 5μL of supernatant was measured by a Pipette and to be diluted to 25mL of solvent. The absorbance was measured by UV-vis (A=0.3499), the diluted concentration c was calculated to be 9.04*10^{-6}mol/L according to the formula $A=\varepsilon d c$ (ε(A=0.3125) =38683) and finally the mass fraction wt% of the saturated solution before dilution were obtained to be 8.50%.

2.3. Solubility test of R-1

Figure S26. Curves of molar extinction coefficient versus concentration for R-1.

To a reactor was added a mixture of 0.20g of R-1 and 0.5mL n-decane, dissolve by ultrasonic stirring 1h, and rest for 2 days. The mixture was centrifuged (10000r/min, 10min)) to remove excess
insoluble dye. 6μL of supernatant was measured by a Pipette and to be diluted to 25mL of solvent. The absorbance was measured by UV- vis (A=0.8426), the diluted concentration c was calculated to be 2.335*10⁻⁵mol/L according to the formula A=ε*d*c (ε(A=2.456)=36837) and finally the mass fraction wt% of the saturated solution before dilution were obtained to be 16.08%.

2.4. Solubility test of C-1

To a reactor was added a mixture of 0.15g of C-1 and 0.5mL n-decane, dissolve by ultrasonic stirring 1h, and rest for 2 days. The mixture was centrifuged (10000r/min, 10min)) to remove excess insoluble dye. 6μL of supernatant was measured by a Pipette and to be diluted to 25mL of solvent. The absorbance was measured by UV- vis (A=0.4931), the diluted concentration c was calculated to be 2.680*10⁻⁵mol/L according to the formula A=ε*d*c (ε(A=0.456)=18405) and finally the mass fraction wt% of the saturated solution before dilution were obtained to be 17.1%.

3. The analysis of the dihedral angle

For the purpose of deep understanding the relation between the molecular structure and the physical properties. Molecular structures of designed dyes were further evaluated by using density functional theory (DFT) at B3LYP/6-31G (d, p) level. The steric effect of two different substituents performs on the perylene core, leads to a twisting conformation for the two naphthalene subunits, and therefore, gives a distorted molecular conformation. The characteristic torsion angles at the bay position of piperidinyl for C-1are 20.18° i and 13.9° ii in phenyloxyl PDI molecules for R-1. torsion angles at the bay position of alkoxy substituents for M-1 is 14.2° , which is nearly similar to R-1. Thus, it is indicated that bigger steric hindrance from piperidinyl groups than that from phenyloxyl and alkoxy groups. This is in accordance with the conclusion deduced from the absorption spectra as mentioned above.
Figure S28. Minimized structures of compounds M-1.
