Electronic Supplementary Material (ESI) for Analyst.

Fluorescent probes based on the isopropylphenyl sulfone encapsulated perylene diimides dyes for imaging of lipid droplets in live Cells

Xinwei Li,[a‡] Zikang Yang,[a‡] Jiqing Bian,[a] Mingyang Fu,[a] Yan Zhang,[a] Nan Jiang,[a] Yanjun Qiao,[a] Hua Chen, [a*] Baoxiang Gao [a, b*]

a. Key Laboratory of Medicinal Chemistry and Molecular Diagnosis (Ministry of Education), College of Chemistry and Environment Science, Hebei University Baoding 071002, P. R. China.

b. Key Laboratory of Analytical Science and Technology of Hebei Province, College of Chemistry and Environment Science, Hebei University Baoding 071002, P. R. China.

‡ These authors contributed equally to this work.

*E-mail: hua-todd@163.com ; bxgao@hbu.edu.cn

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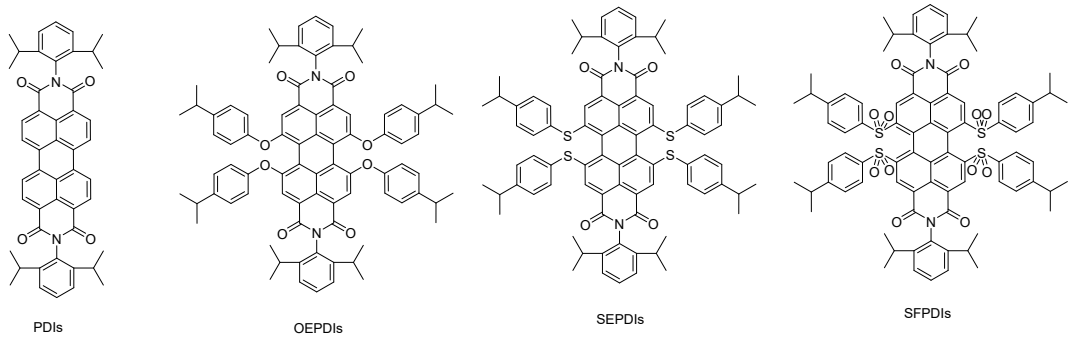
Part A: Experimental Section

1 General information on materials

The chemical reagents were purchased from J&K Scientific Ltd or Beijing zhong sheng hua teng Technology Co., Ltd. and used as received. Solvents were either employed as purchased or dried according to procedures described in the literature. Deionized water was obtained from a Milli-Q water purification system (Millipore). Phosphate buffer saline (PBS) was purchased from Life Technologies Co., Ltd.. All glassware was oven-dried prior to use when water- and/or air-sensitive reagents were used. The synthetic steps were performed under ambient atmosphere unless stated otherwise. The ^{1}H-NMR spectra were recorded at 20°C on 600 MHz or 400MHz NMR spectrometer (Bruker). The ^{13}C-NMR spectra were recorded at 20°C on 150 MHz or 101 MHz NMR spectrometer (Bruker). Mass spectra were carried out using Thermo Finnigan TSQ Quantum Ultra AM EMR Mass Spectrometry or ApexUltra Fourier transform ion cyclotron resonance mass spectrometry (Bruker). Cyclic voltammetry (CV) was performed on a CHI660b electrochemical ananlyzer with a three-electrode cell in 0.1 M tetrabutylammoniumperchlorate (Bu_4NClO_4) dichloromethane solution at a scan rate of 100 mV/s. A glass carbon disk (2-mm diameter) was used as working electrode with a Pt wire as the counter electrode and an Ag/AgCl electrode as the reference electrode. The redox potential was calibrated with ferrocene/ferrocenium (0.438 V *vs* Ag/AgCl in DCM). Energy gap (E_g) and

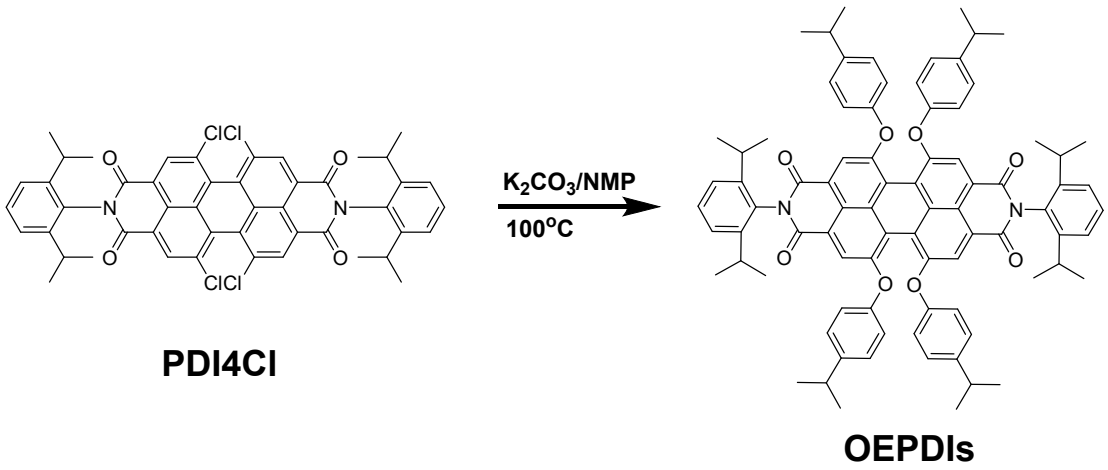
LUMO energy levels were calculated according to E_g=1240/λ_{onset} and LUMO=–(4.38+E^{onset}_{red}), respectively. UV/Vis spectra were recorded with a Shimadzu WV-2550 spectrophotometer. Fluorescence spectra were recorded on a Shimadzu RF-5301 fluorescence spectrophotometer. Fluorescence quantum yield was determined using optically matching solutions of PDIs (Φ = 100, in DCM) as the standard at an excitation wavelength of 646 nm and the quantum yield was calculated using the following equation: $\Phi s = \Phi_r (A_r F_s / As\ F_r) (n_s^2/n_r^2)$, where, s and r denote sample and reference, respectively, A is the absorbance, F is the relative integrated fluorescence intensity, and n is the refractive index of the solvent. Fluorescence microscopy images of labelled cells were obtained with spectral confocal laser scanning microscopy (Olympus Fluoview FV-1000).

2 Synthesis and characterization of PDI dyes



Scheme S1. Chemical structure of PDIs dyes

Synthesis of OEPDIs



PDI4Cl (100mg, 0.118mmol), anhydrous potassium carbonate (81.4 mg, 0.590 mmol), and 4-Isopropylphenol (170 mg, 1.250 mmol) were mixed in 15 mL N-Methyl pyrrolidone. The mixture was heated to 80 °C for 15 h, the solution was cooled to room temperature, the mixture was poured into 50 mL of 2 M hydrochloric acid to precipitate the product, washed with water to neutrality, and dried in vacuum. The crude product was further purified by column chromatography (Dichloromethane/Petroleum ether = 1:2) to afford OEPDIs (red solid, 32 mg, yield 22%). ^{1}H NMR(600 MHz，CDCl3) δ(ppm)：8.32(s，4H)，7.46(t，J =7.8Hz，2H)，7.30(t，J =7.8Hz，4H)，7.13(d，J =8.4 Hz，8H)，6.92(d，J =9.0 Hz，8H)，2.88(m，4H)，2.74(m，4H)，1.25(d，J =7.2 Hz，24H)，1.16(d，J =6.6 Hz，24H).

3 Supplementary Figures

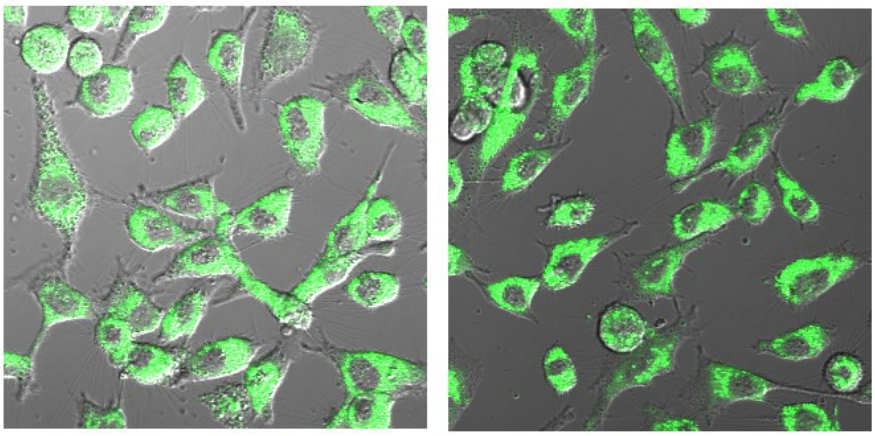


Figure S1. Cell enzymatic activity assay. After being exposed to 20 μM **SFPDIs** for 24 h, the cells were incubated for an extra 30 min in standard culture media containing calcein AM and imaged again. Calcein AM is a common cell-permeant dye used to determine cell viability in most eukaryotic cells. In live cells the non-fluorescent calcein AM is converted to a green-fluorescent calcein after acetoxymethyl ester hydrolysis by intracellular esterases.

Part B: ^{1}H-NMR spectrum, ^{13}C NMR spectrum and MS spectrum

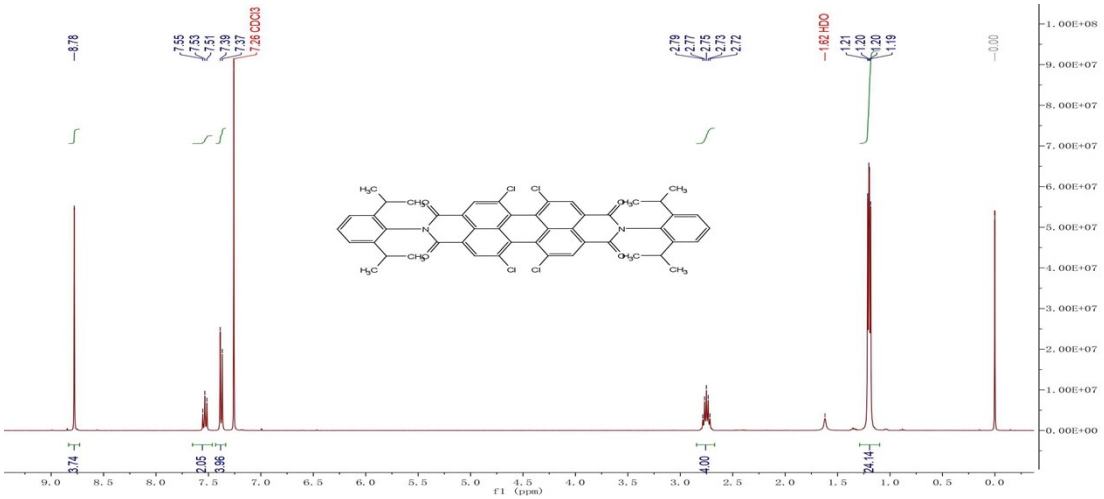


Figure S2 ^{1}H NMR (400 MHz) spectra of PDI4Cl in $CDCl_3$

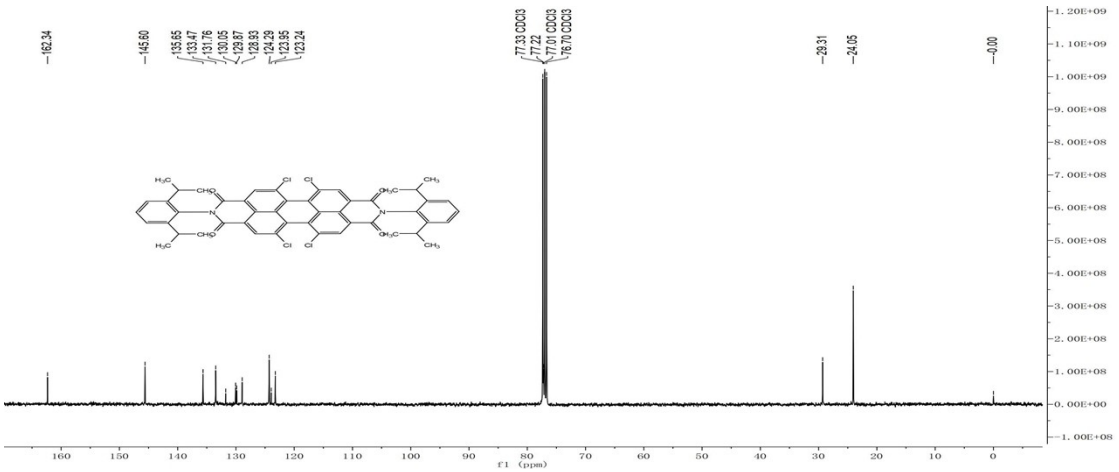


Figure S3 ^{13}C NMR (101 MHz) spectra of PDI4Cl in $CDCl_3$

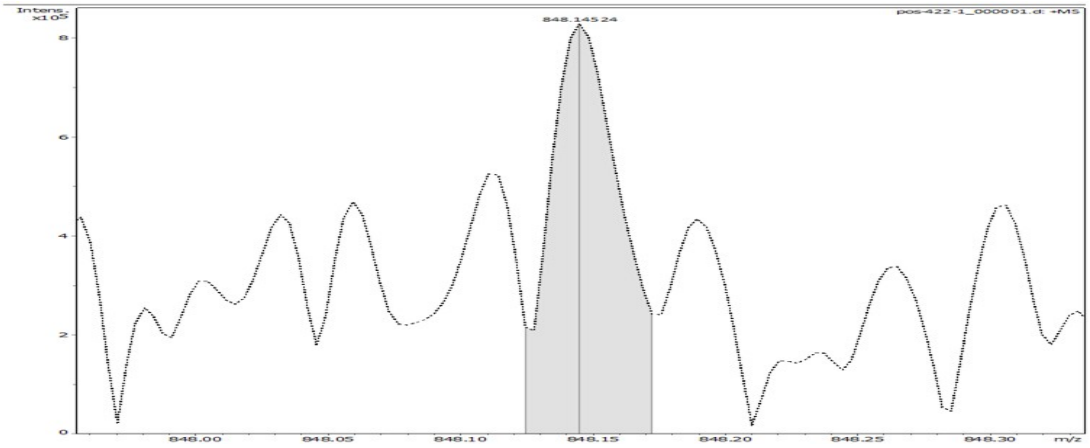


Figure S4 MS spectrum of PDI4Cl

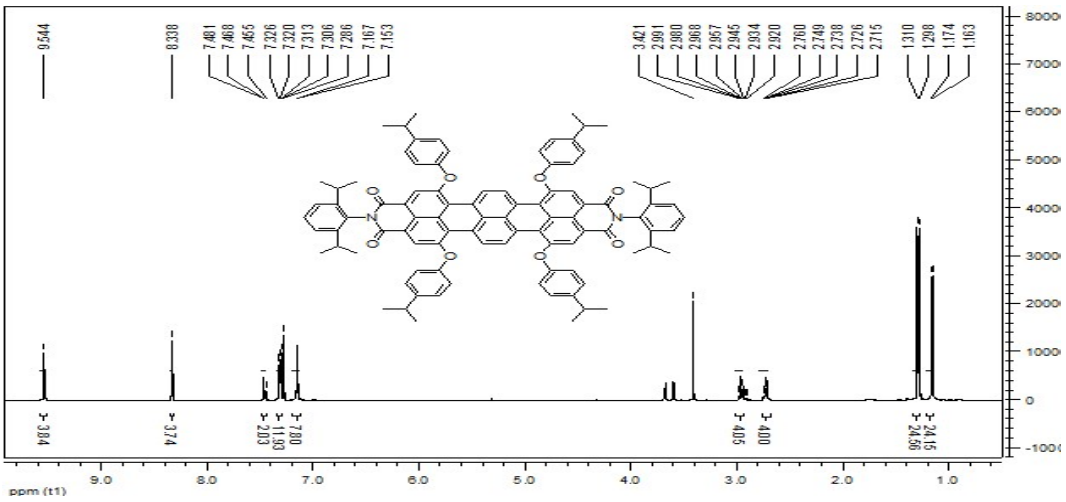


Figure S5 ^{1}H NMR (600 MHz) spectra of OEPDIs in $CDCl_3$

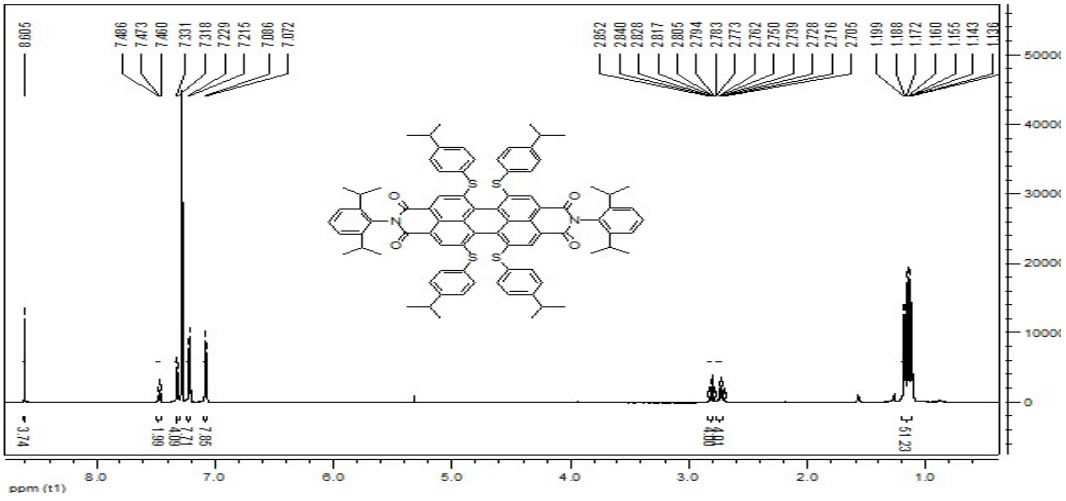


Figure S6 ^{1}H NMR (600 MHz) spectra of SEPDIs in $CDCl_3$

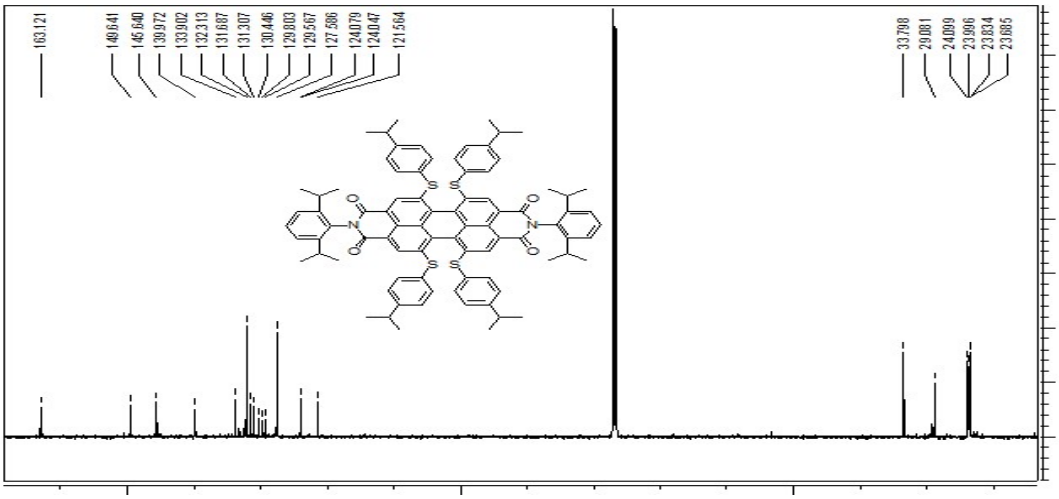


Figure S7 ^{13}C NMR (150 MHz) spectra of SEPDIs in $CDCl_3$

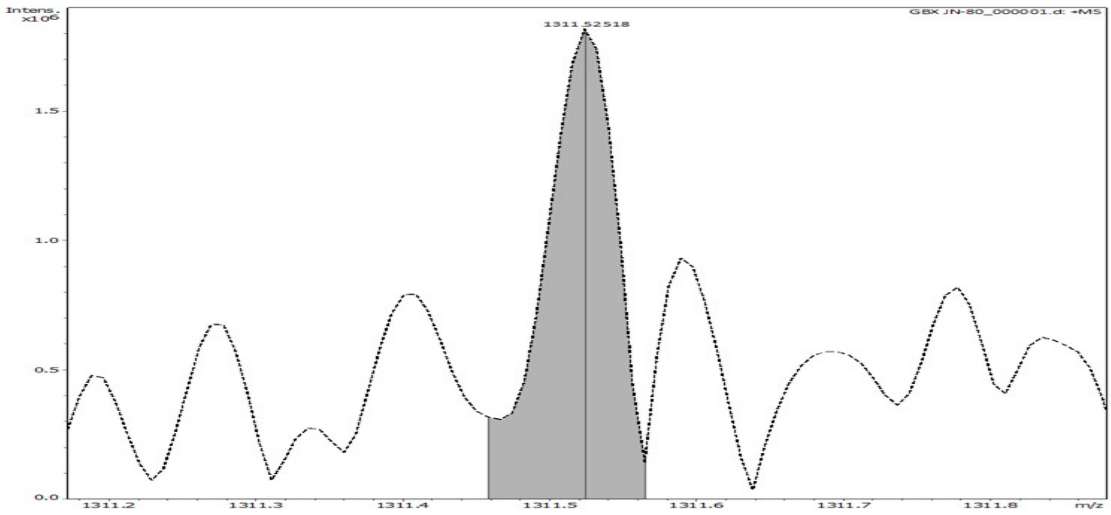


Figure S8 MS spectrum of SEPDIs

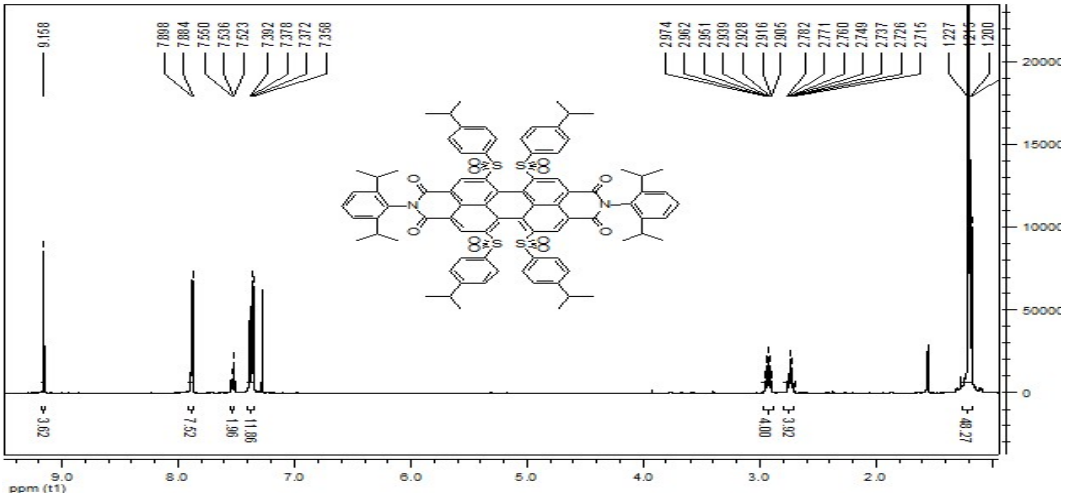


Figure S9 ^{1}H NMR (600 MHz) spectra of SFPDIs in $CDCl_3$

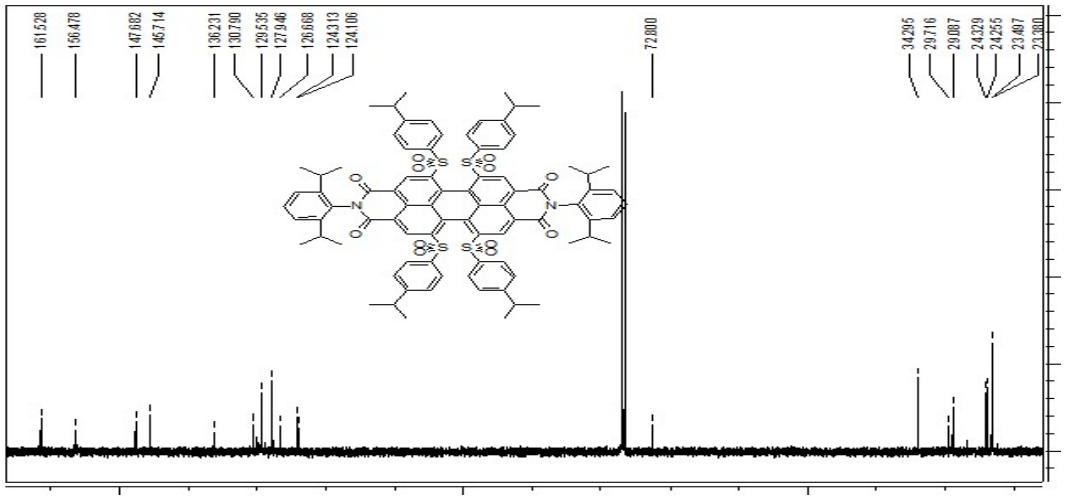


Figure S10 ^{13}C NMR (150 MHz) spectra of SFPDIs in $CDCl_3$

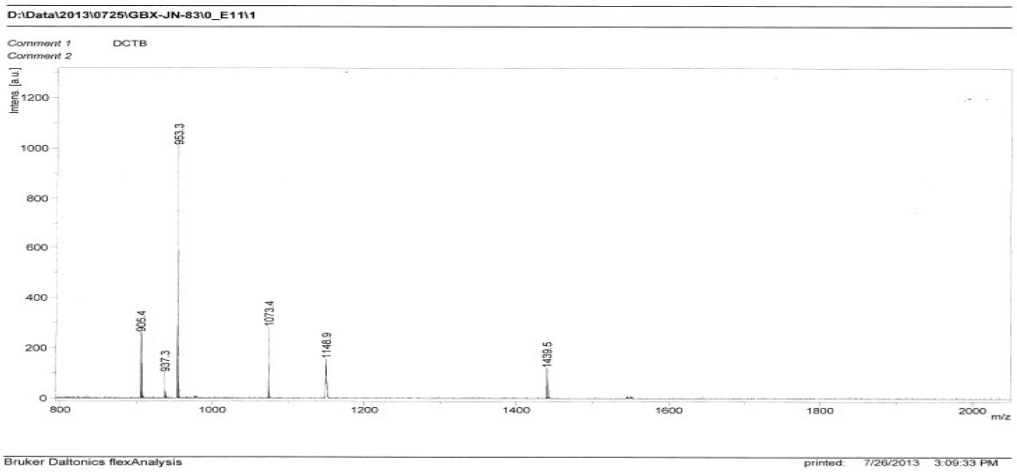


Figure S11 MS spectrum of SFPDIs