Electronic Supplementary Information (ESI) for

Diacenopentalene dicarboximides as new n-type organic semiconductors for field effect transistors

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1. DFT calculation details

DFT calculations have been performed at the B3LYP/6-31G*[1-5] level of theory, as implemented in the Gaussian 09 program package.[6] Absorption spectra of **DBPDI** and **DNPDI** were calculated by TD DFT at B3LYP/6-31G* level.

Table S1. Selected TD-DFT (B3LYP/6-31G*) calculated energies, oscillator strength and compositions of major electronic transitions of **DBPDI**.

Wavelength (nm)	Osc. Strength (*f*)	Major contributions
614.0	0.0000	HOMO->LUMO (99%)
488.2	0.3379	H-1->LUMO (94%)
364.5	0.1160	H-5->LUMO (72%), HOMO->L+1 (10%)
351.8	0.1938	H-5->LUMO (10%), HOMO->L+1 (78%)
300.4	0.1959	H-13->LUMO (63%), H-1->L+2 (27%)
292.3	1.2580	H-1->L+2 (15%), HOMO->L+3 (57%)

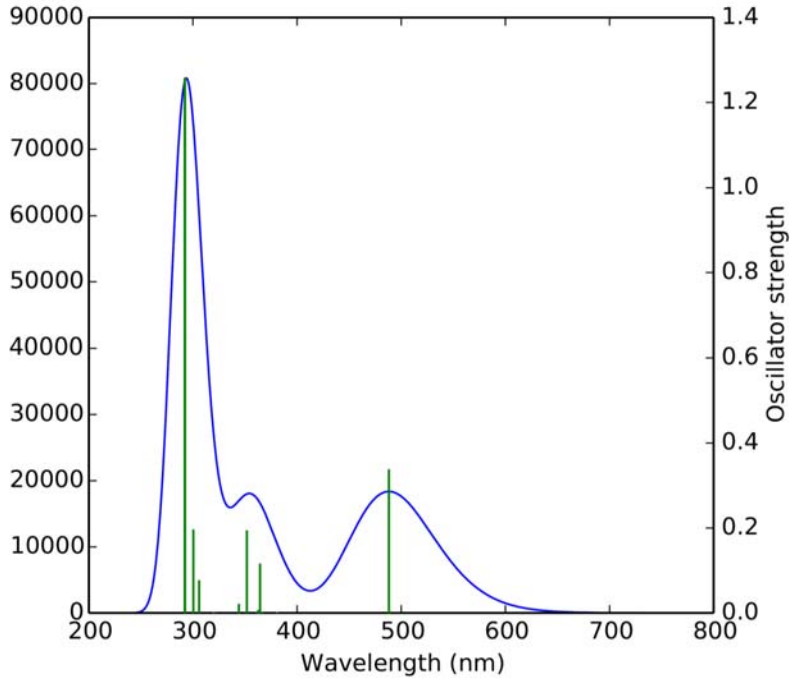

Figure S1. Calculated (B3LYP/6-31G*) absorption spectrum of **DBPDI**.

Table S2. Selected TD-DFT (B3LYP/6-31G*) calculated energies, oscillator strength and compositions of major electronic transitions of **DNPDI**.

Wavelength (nm)	Osc. Strength (*f*)	Major contributions
512.3	0.5057	HOMO->LUMO (92%)
364.8	0.2907	H-3->LUMO (72%), H-1->L+1 (18%)
352.2	0.6585	H-1->L+1 (43%), HOMO->L+3 (18%), HOMO->L+4 (20%)
334.3	0.5457	H-6->LUMO (18%), H-1->L+1 (14%), H-1->L+2 (21%), HOMO->L+3 (10%), HOMO->L+4 (27%)
332.4	0.4603	H-8->LUMO (12%), H-6->LUMO (39%), H-1->L+2 (12%), HOMO->L+4 (18%)
330.2	0.1145	H-8->LUMO (86%)
328.2	0.7654	H-6->LUMO (13%), H-3->LUMO (10%), H-1->L+2 (29%), HOMO->L+3 (18%), HOMO->L+4 (13%)

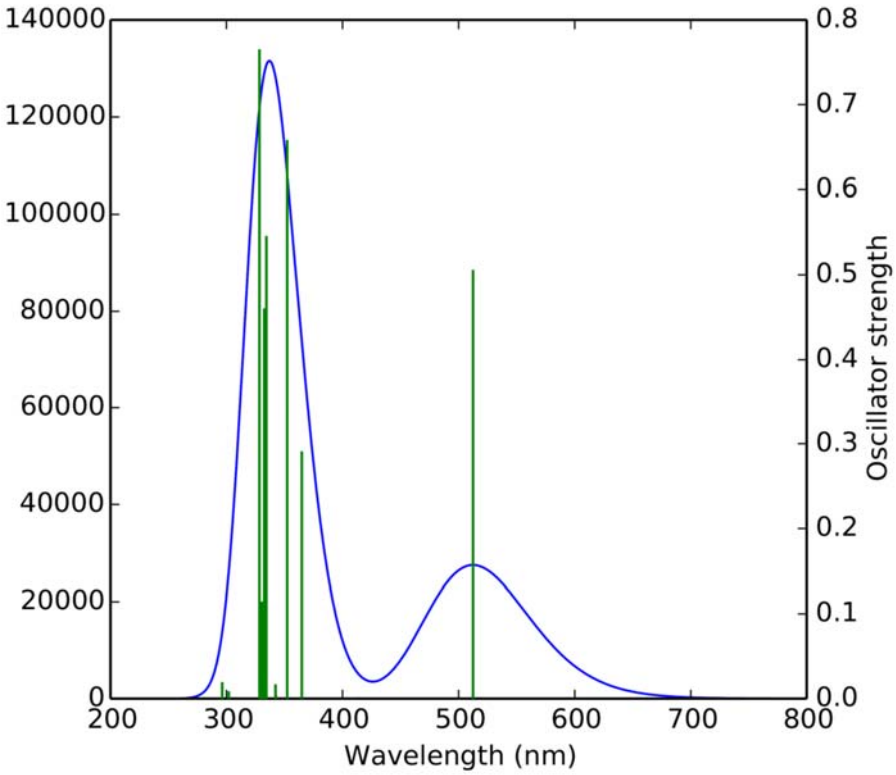

Figure S2. Calculated (B3LYP/6-31G*) absorption spectrum of **DNPDI**.

References:

1. Becke, A. D. *J. Chem. Phys.***1993**, *98*, 5648.
2. Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B: Condens. Matter***1988**, *37*, 785.
3. Ditchfie, R. W.; Hehre, J.; Pople, J. A. *J. Chem. Phys.***1971**, *54*, 724.
4. Hehre, W. J.; Ditchfie R.; Pople, J. A. *J. Chem. Phys.***1972**, *56*, 2257.
5. Harihara, P. C.; Pople, J. A. *Theor. Chim.Acta***1973**, *28*, 213.
6. *Gaussian 09; Revision A.2*; Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian, Inc., Wallingford CT, 2009.

2. Differential pulse voltammograms

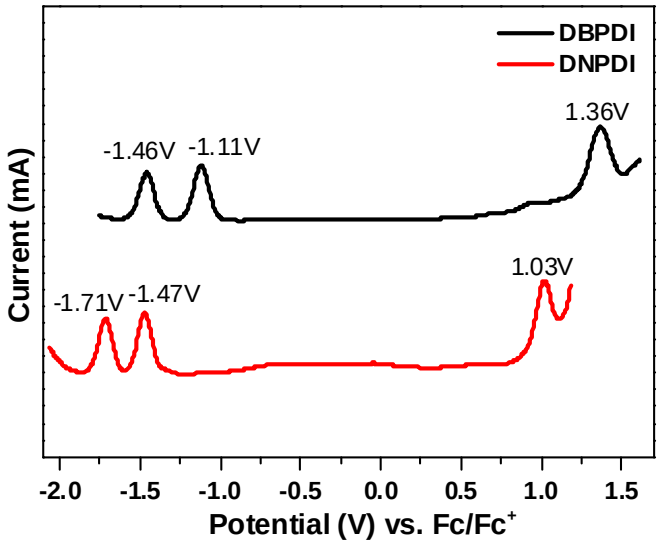

Figure S3 Differential pulse voltammograms (1×10^{-3}M) of compounds **DBPDI** and **DNPDI** in dry dichloromethane with 0.1 M Bu_4NPF_6 as the supporting electrolyte, AgCl/Ag as reference electrode, Au as working electrode(surface area = 12.6 mm^2), Pt wire as counter electrode (potential step = 0.004 V, pulse amplitude = 0.05 V, pulse width = 0.05 s in the oxidation mode).

3. TGA and DSC curves

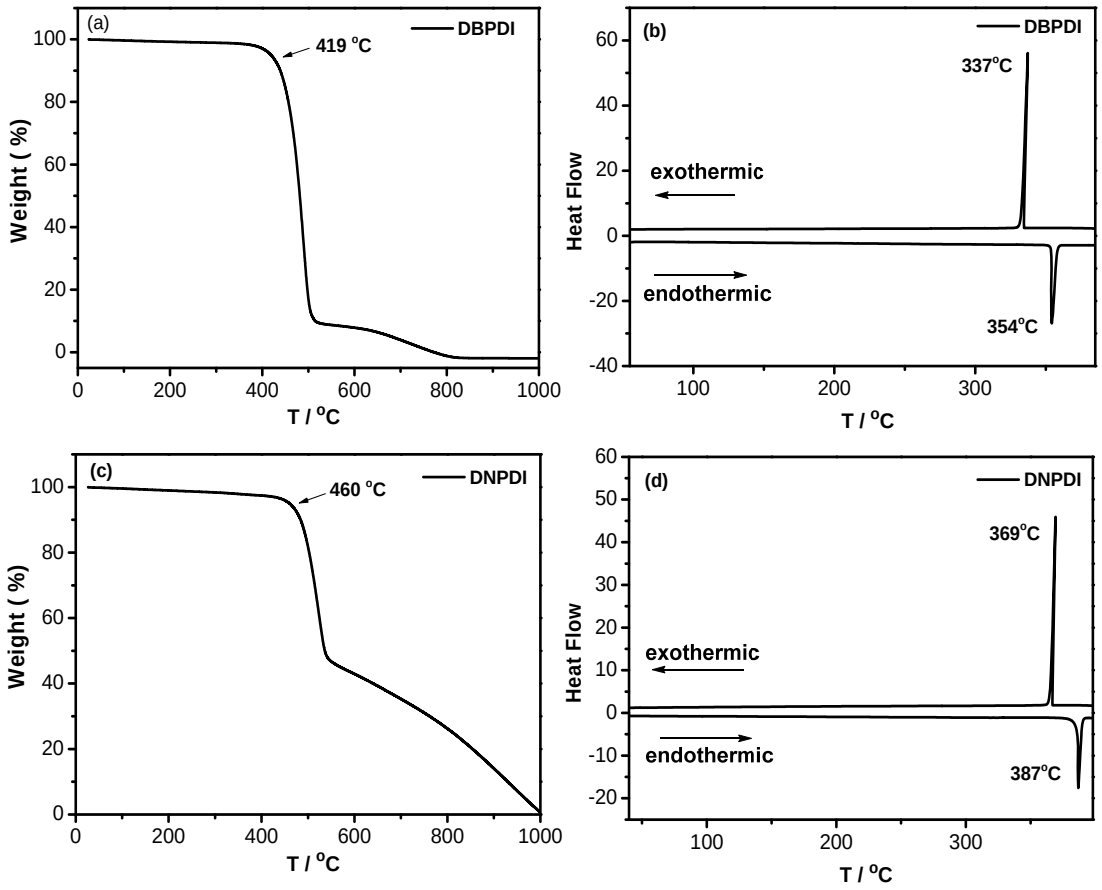

Figure S4 Thermogravimetric analysis (TGA) of compounds **DBPDI** (a) and **DNPDI** (c); Differential scanning calorimetry (DSC) of compounds **DBPDI** (b) and **DNPDI** (d) in N_2 at a heating rate of 10 $^oC\ min^{-1}$

6. NMR spectra of all new compounds

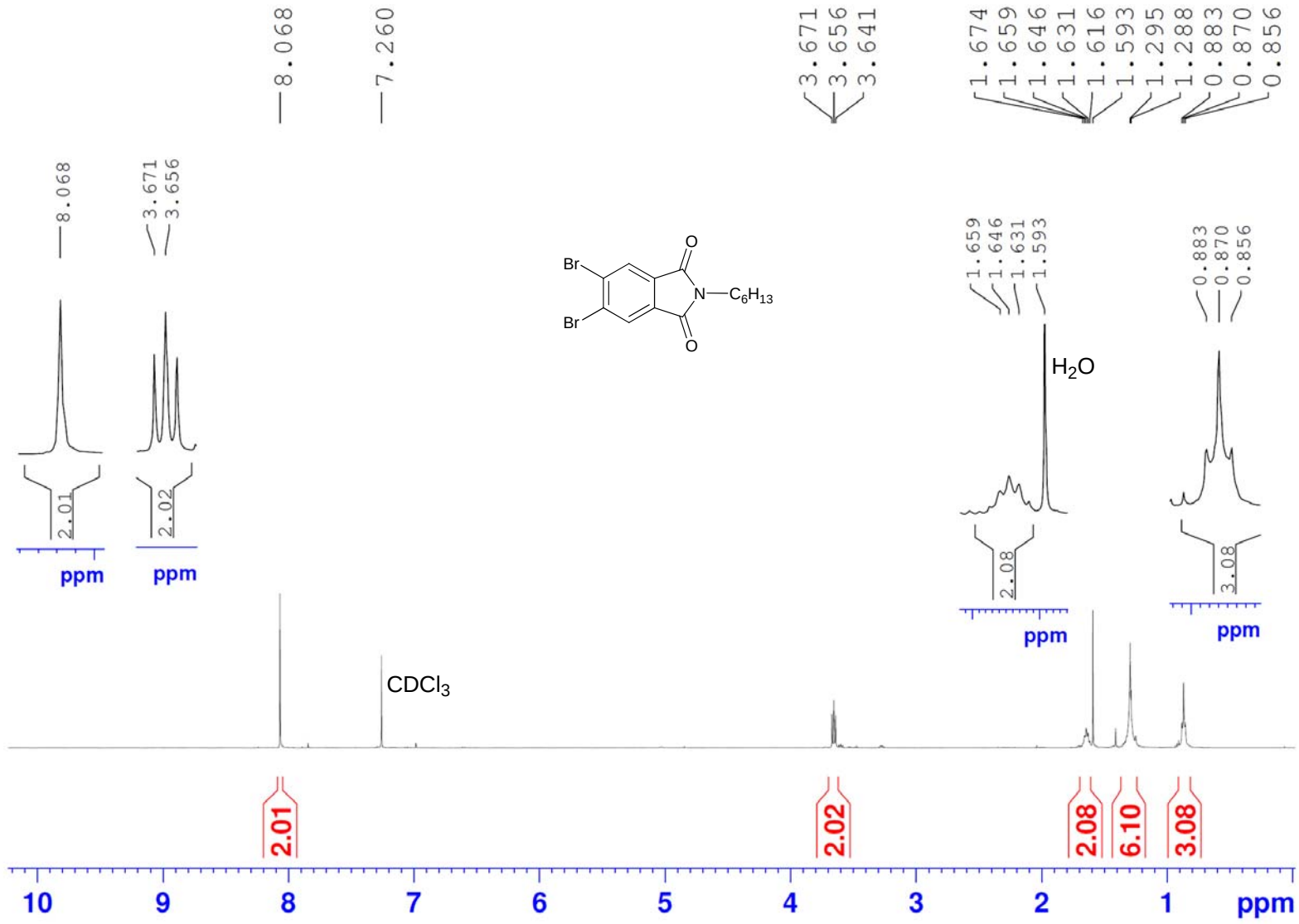

Figure S5 ^{1}H NMR (500 MHz) spectrum of compound **2** in $CDCl_3$

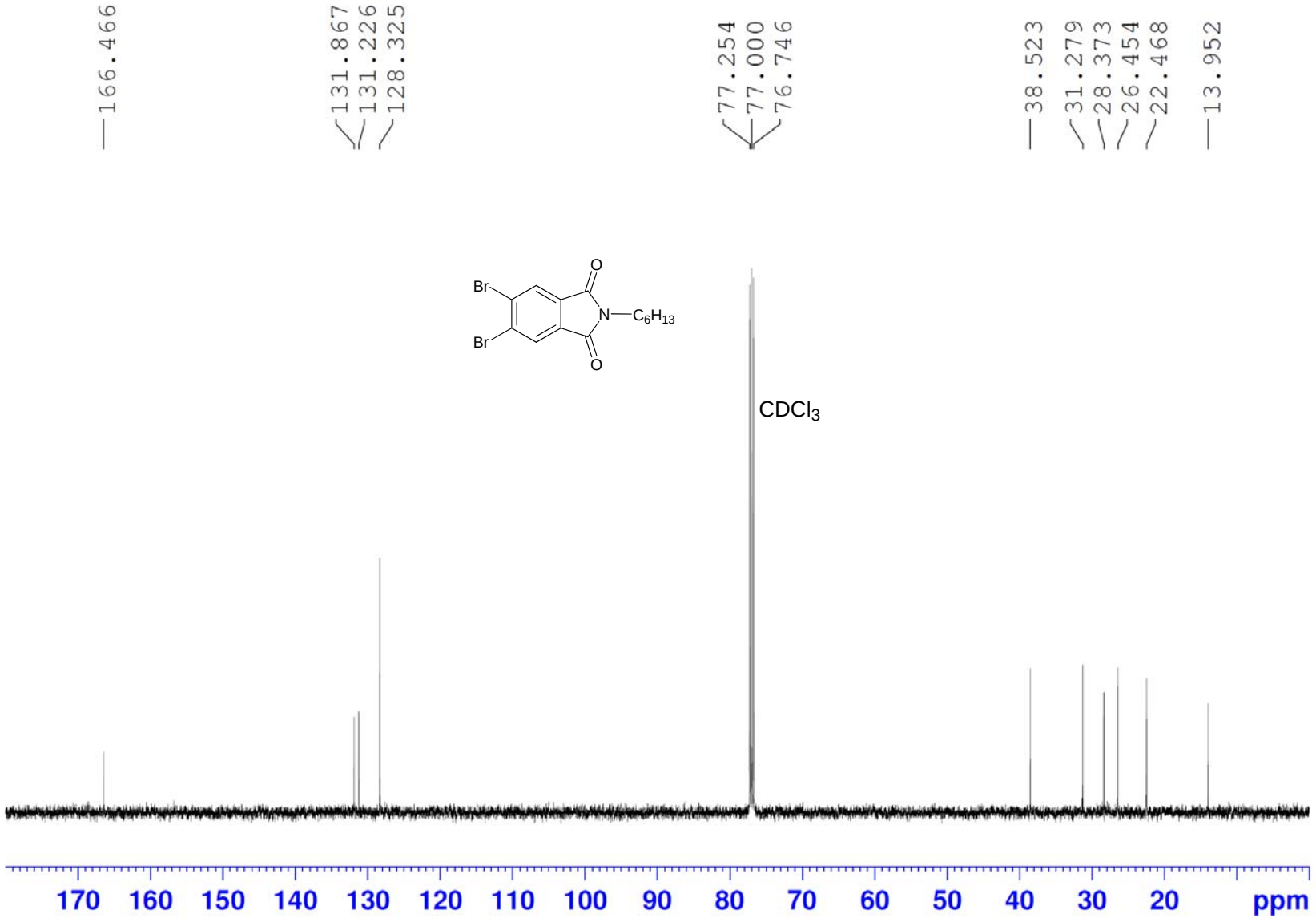

Figure S6 ^{13}C NMR (125 MHz) spectrum of compound **2** in $CDCl_3$

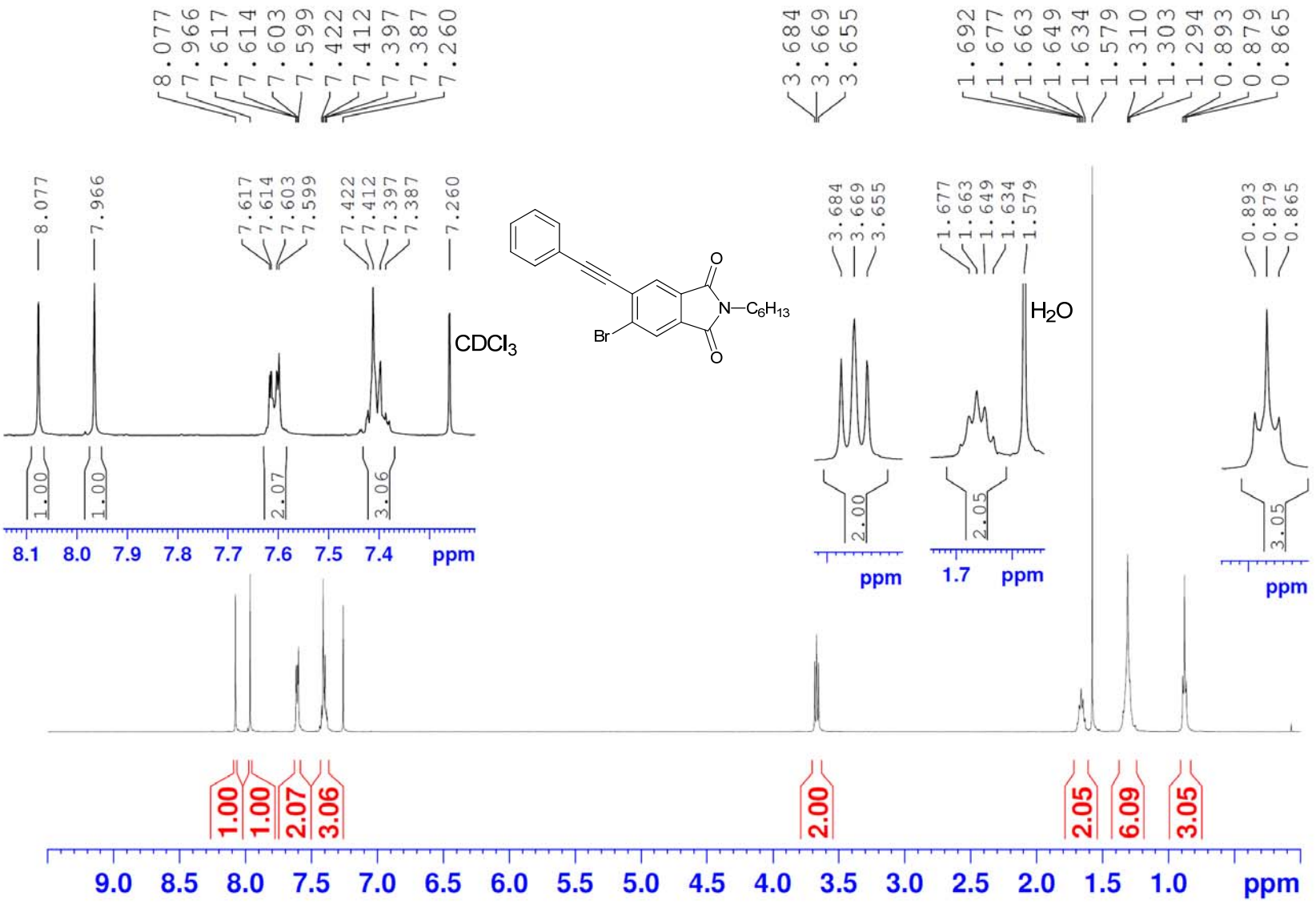

Figure S7 ^{1}H NMR (500 MHz) spectrum of compound **3** in $CDCl_3$

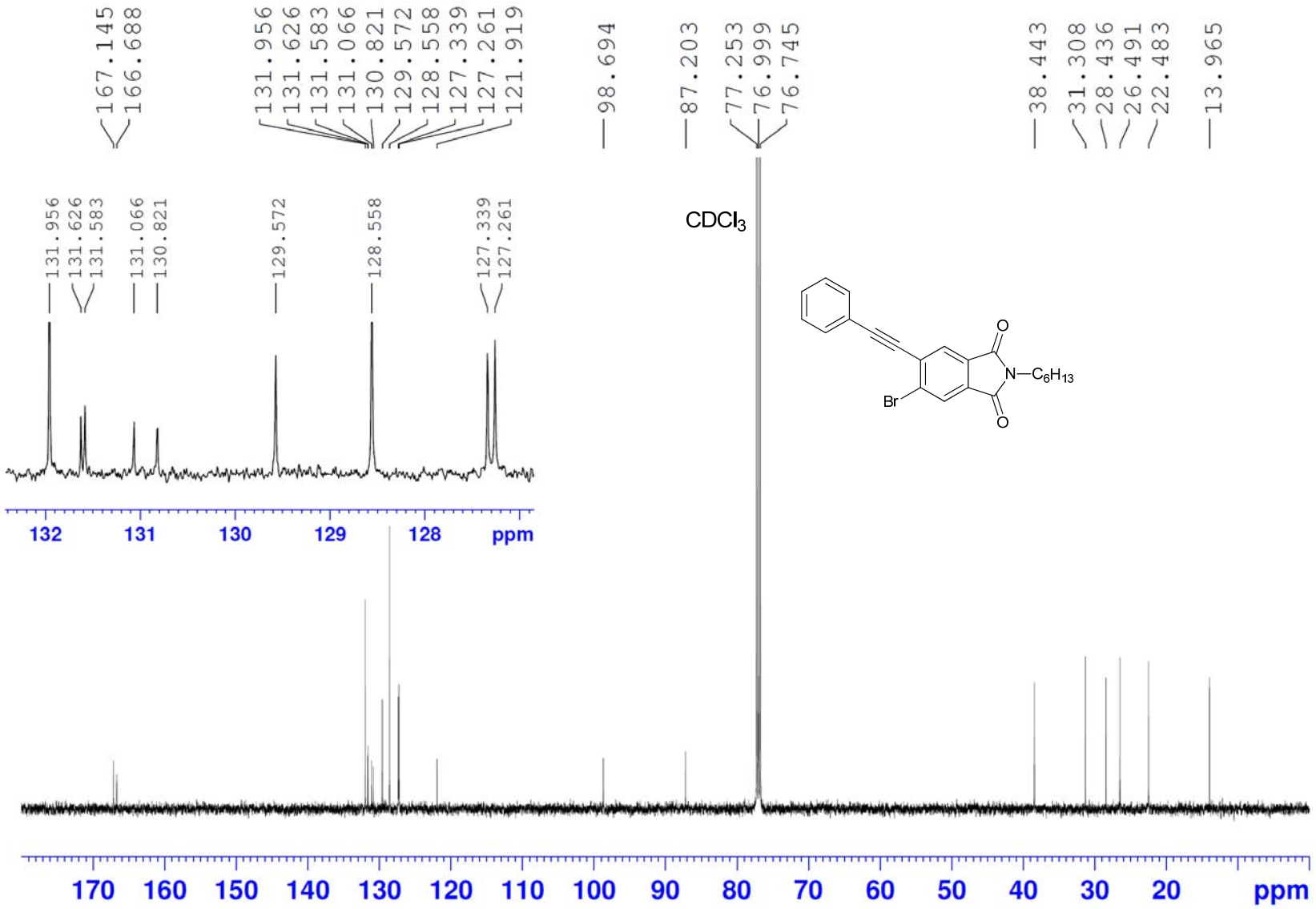

Figure S8 ^{13}C NMR (125 MHz) spectrum of compound **3** in $CDCl_3$

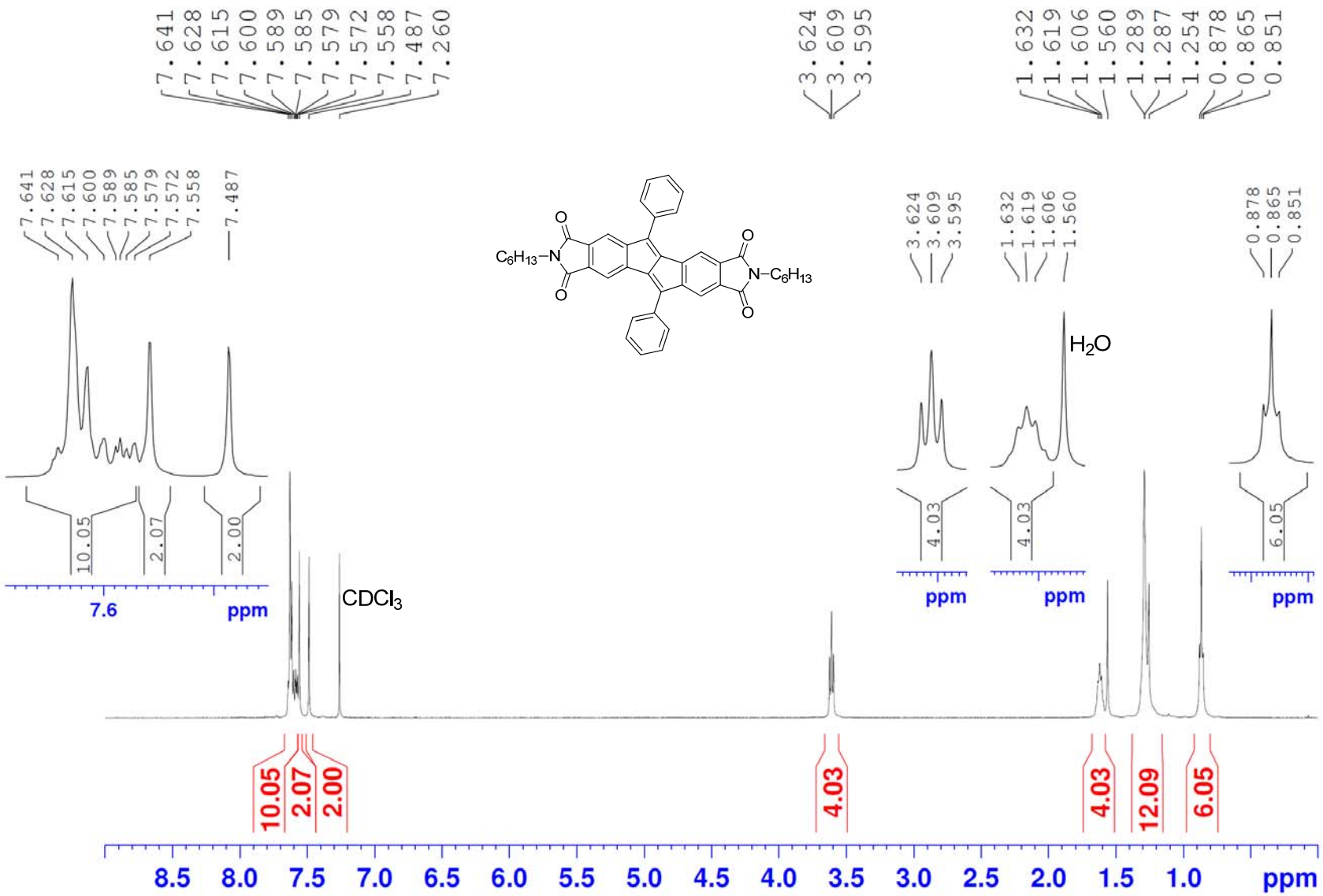

Figure S9 ^{1}H NMR (500 MHz) spectrum of compound **DBPDI** in $CDCl_3$

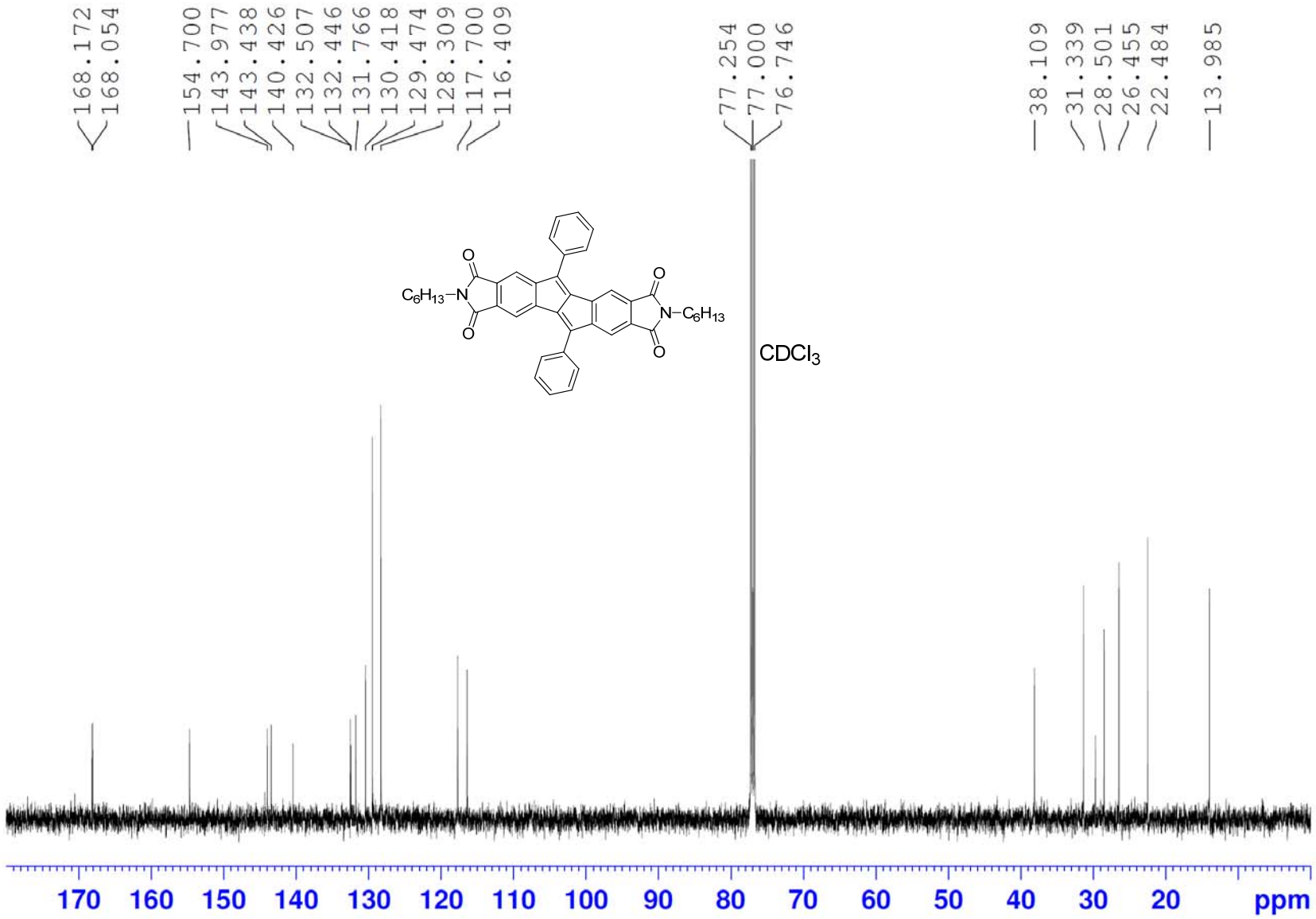

Figure S10 ^{13}C NMR (125 MHz) spectrum of compound **DBPDI** in $CDCl_3$

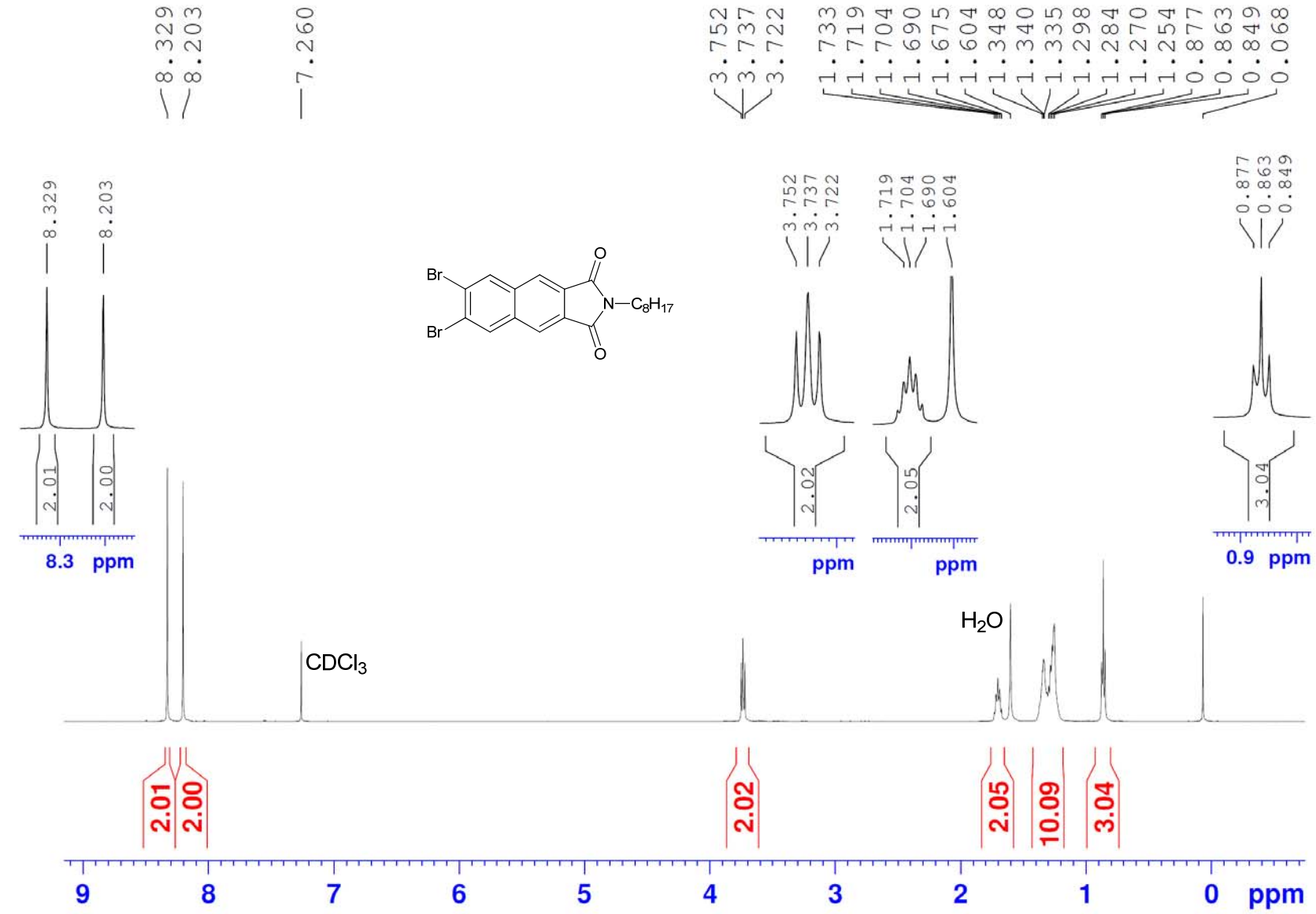

Figure S11 ^{1}H NMR (500 MHz) spectrum of compound **6** in $CDCl_3$

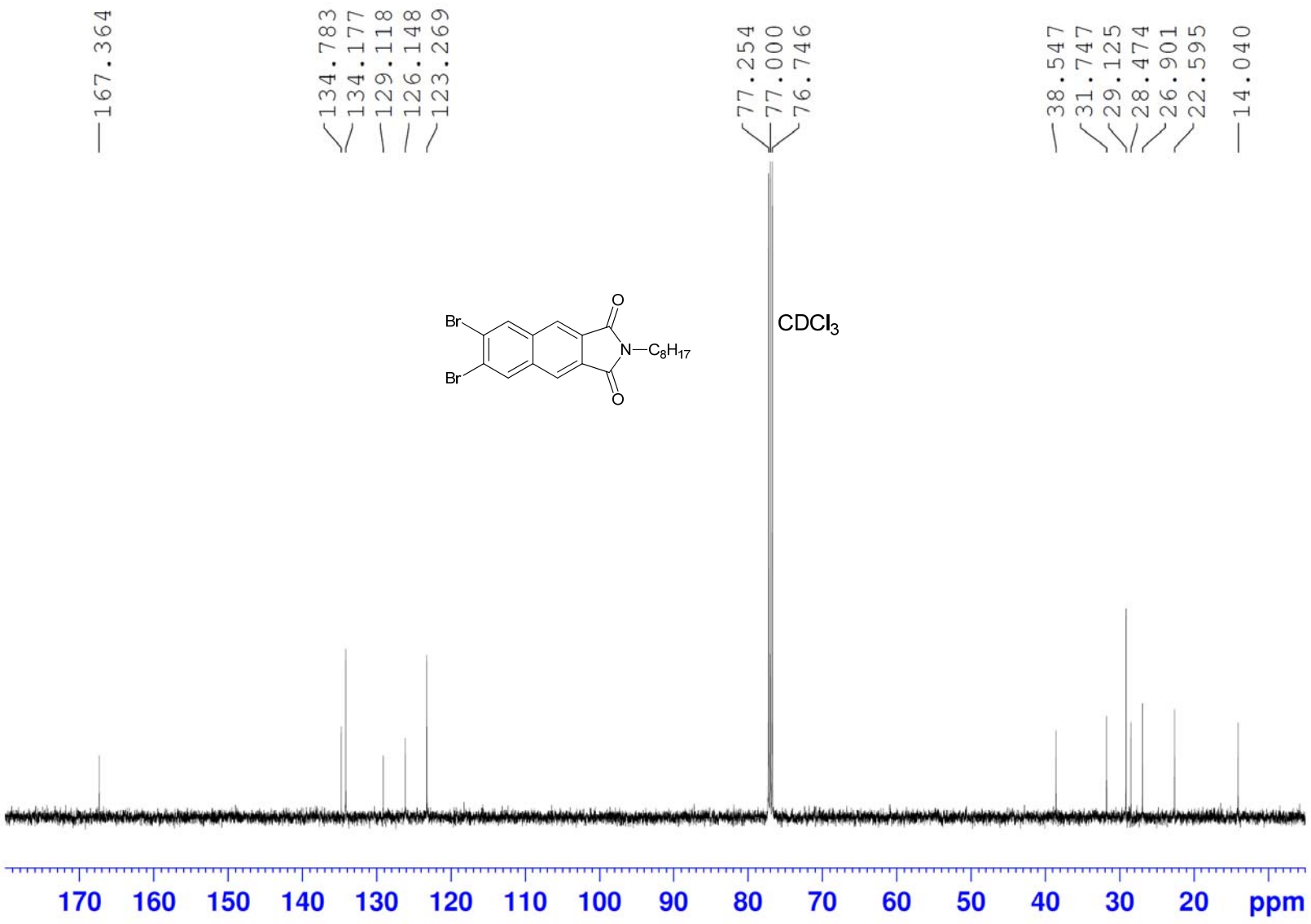

Figure S12 ^{13}C NMR (125 MHz) spectrum of compound **6** in $CDCl_3$

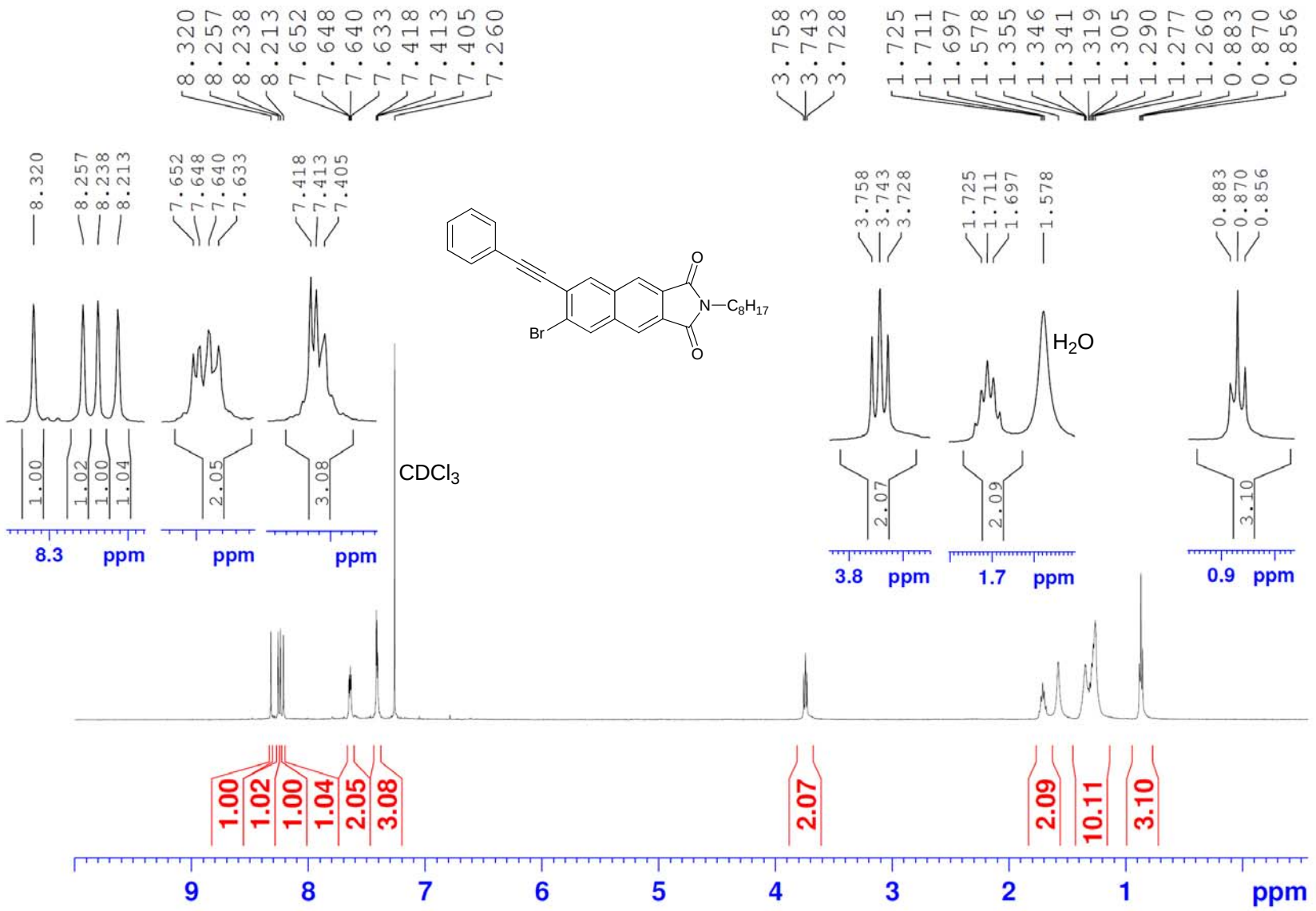

Figure S13 ^{1}H NMR (500 MHz) spectrum of compound **7** in $CDCl_3$

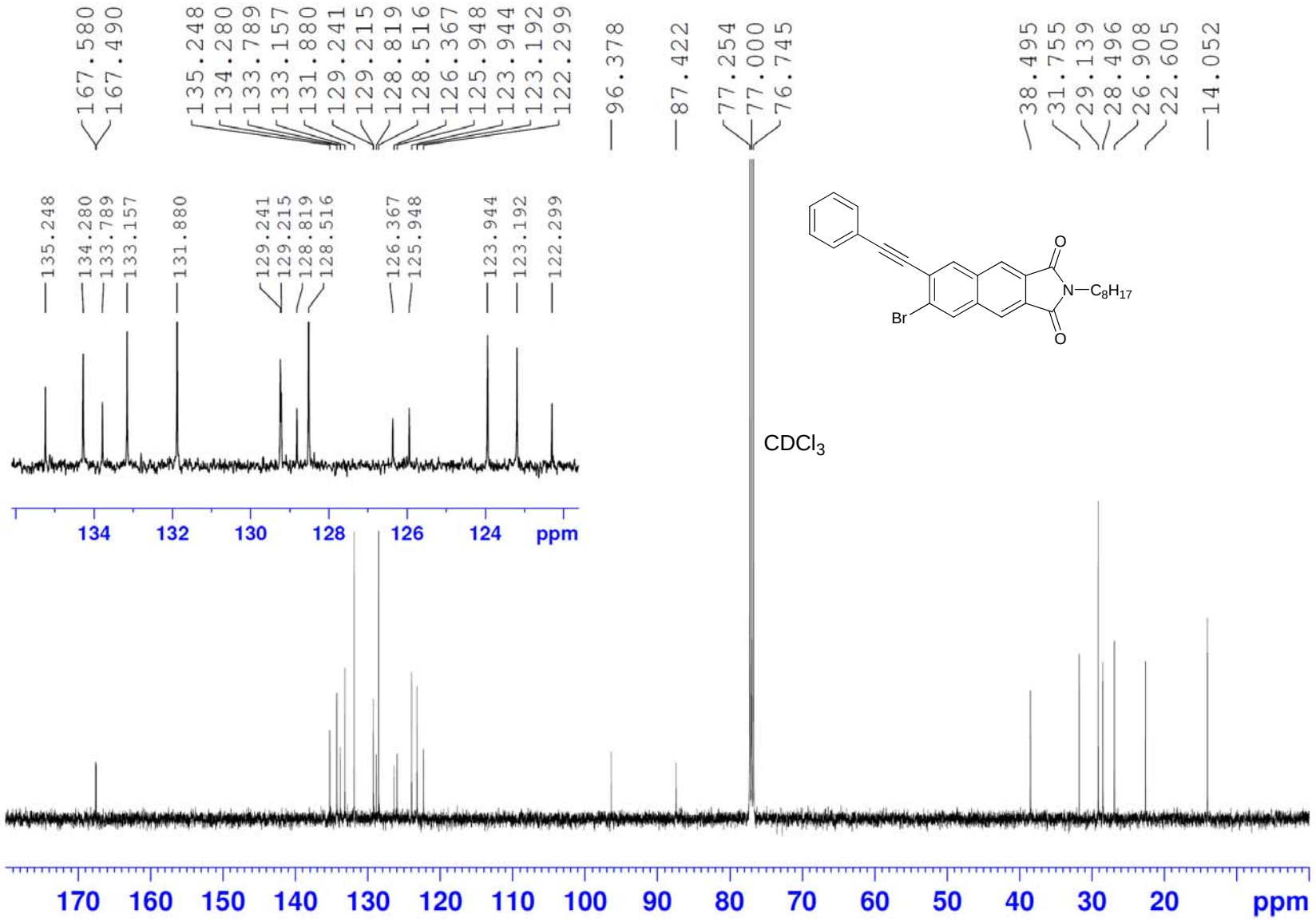

Figure S14 ^{13}C NMR (125 MHz) spectrum of compound **7** in $CDCl_3$

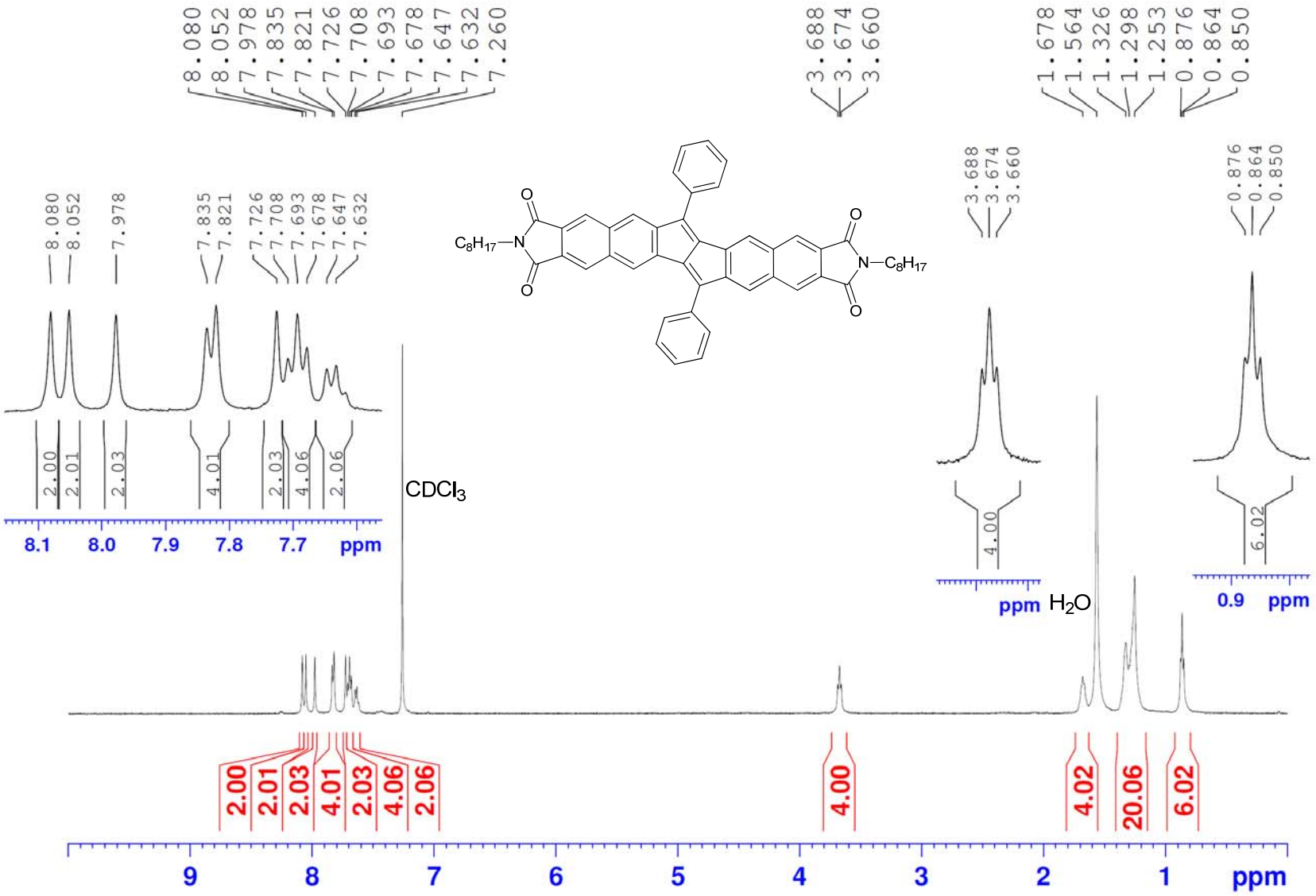

Figure S15 ^{1}H NMR (500 MHz) spectrum of compound **DNPDI** in $CDCl_3$

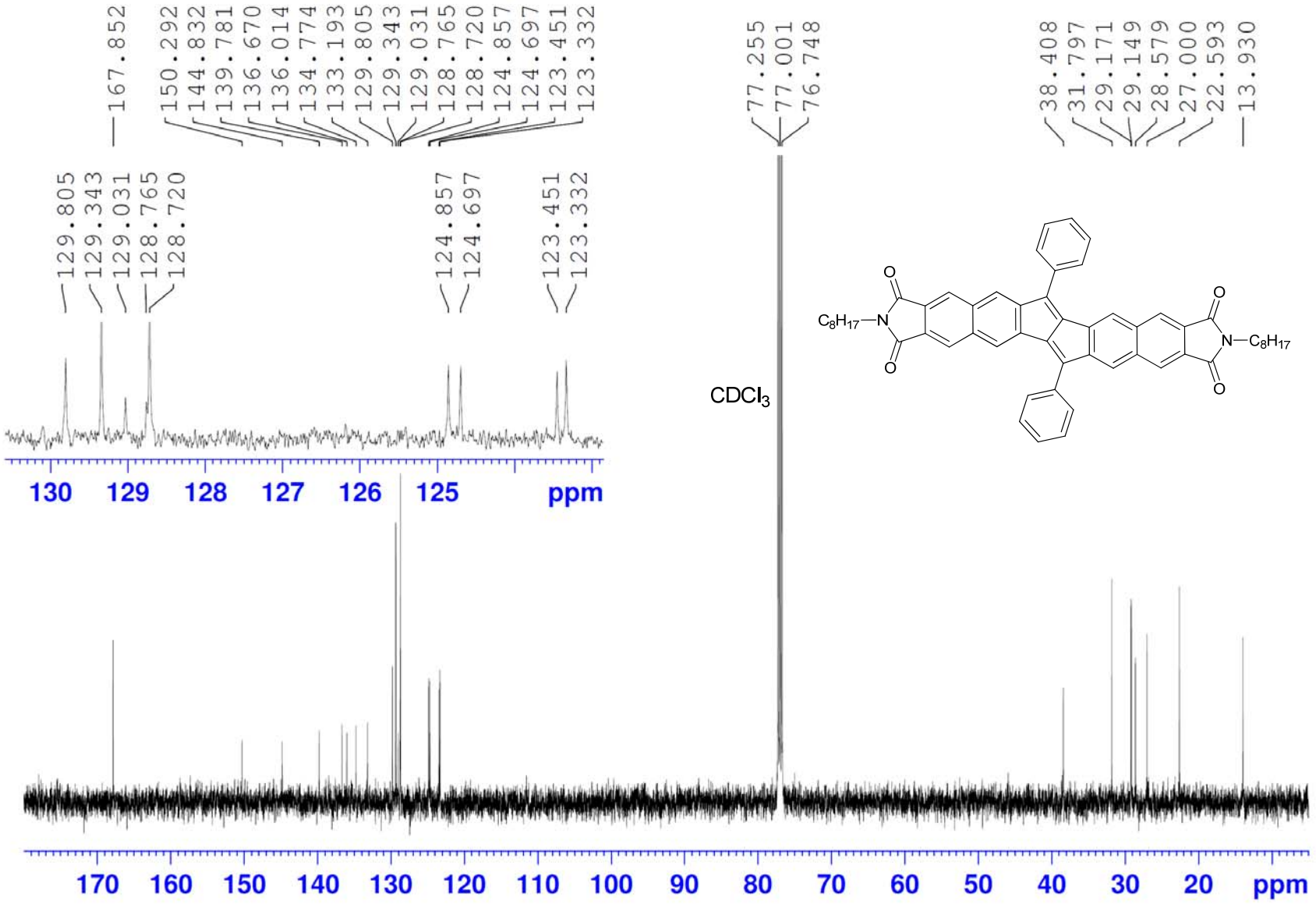

Figure S16 ^{13}C NMR (125 MHz) spectrum of compound **DNPDI** in $CDCl_3$