Electronic Supporting Information For

Pyrrolophthalazine Dione (PPD)-based Donor-Acceptor Polymers as High Performance Electrochromic Materials

Qun Ye,[+,a] Wei Teng Neo,[+,a,b] Tingting Lin,[a] Jing Song,[a] Hong Yan,[a] Hui Zhou,[a] Kwok Wei Shah,[a] Soo Jin Chua,[a,c] and Jianwei Xu[a,d,*]

[a] Institute of Materials Research and Engineering, A*STAR, 3 Research Link, Singapore 117602.

[b] NUS Graduate School for Integrative Sciences and Engineering, National University of Singapore, 28 Medical Drive, Singapore 117456.

[c] Department of Electrical and Computer Engineering, National University of Singapore, 4 Engineering Drive 3, Singapore 117583

[d] Department of Chemistry, National University of Singapore, 3 Science Drive 3, Singapore 117543

[+] These authors contribute equally to this work.

Contents

1. Spectroelectrochemical graphs of P1 and P3 devices……2

2. Switching behavior of P1 and P3 devices……3

3. Redox stability of P2 device d P3 devices……4

4. TD-DFT calculations details……5

5. NMR spectra of all new compounds……7

1. Spectroelectrochemical graphs of P1 and P3 devices

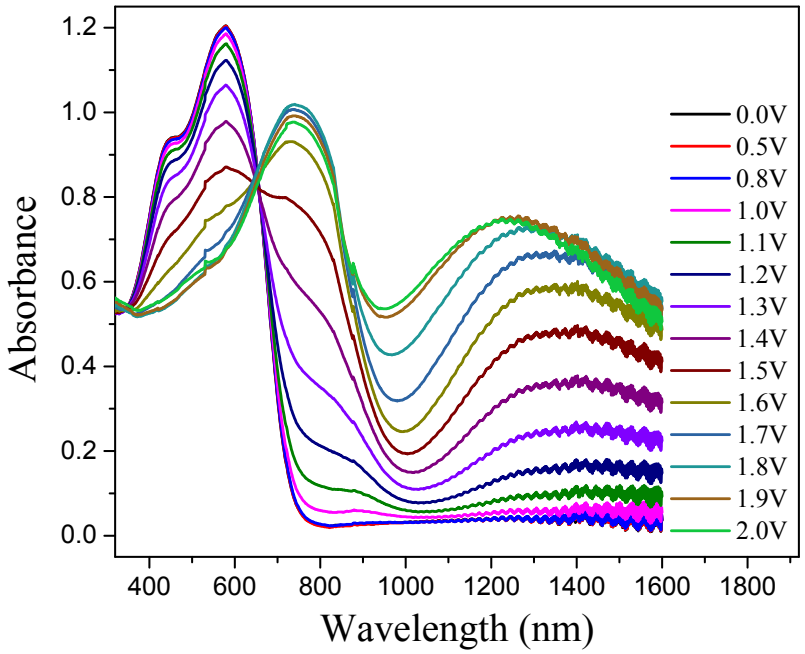


Fig. S1 Spectroelectrochemical graphs of drop-cast **P1** device at various applied potentials.

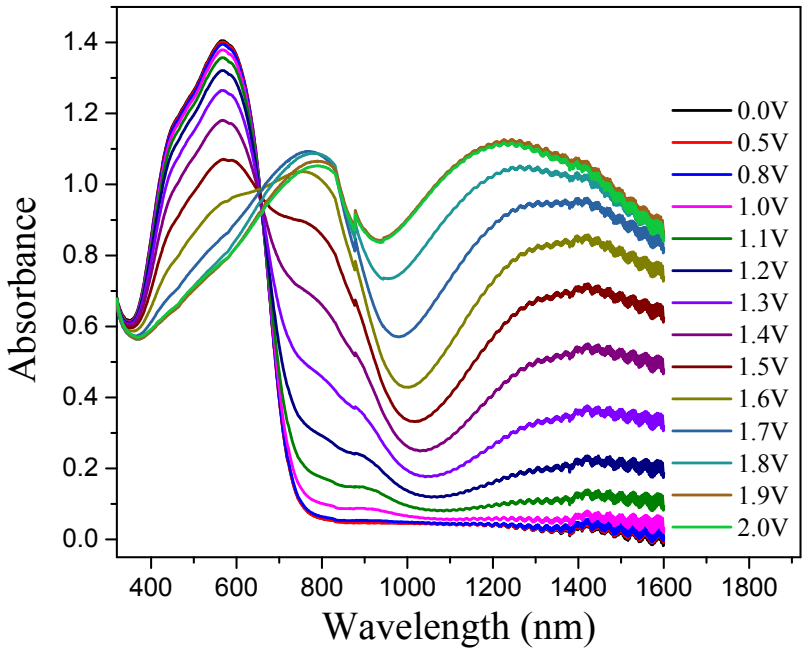


Fig. S2 Spectroelectrochemical graphs of drop-cast **P3** device at various applied potentials.

2. Switching behavior of P1 and P3 devices

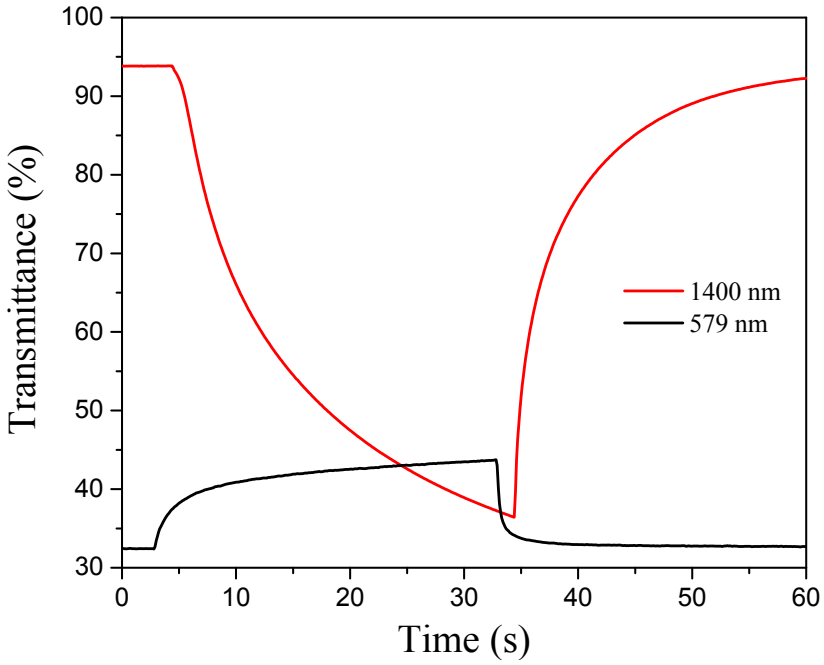


Fig. S3 Switching behaviour of **P1** device between + 1.6 and -1.6 V.

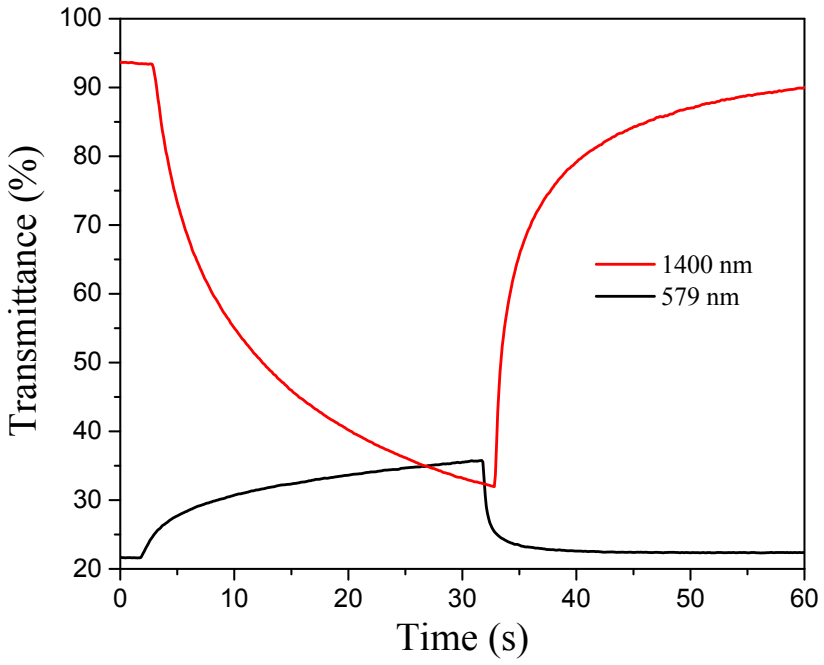


Fig. S4 Switching behaviour of **P3** device between + 1.6 and -1.6 V.

3. Redox stability of P2 device

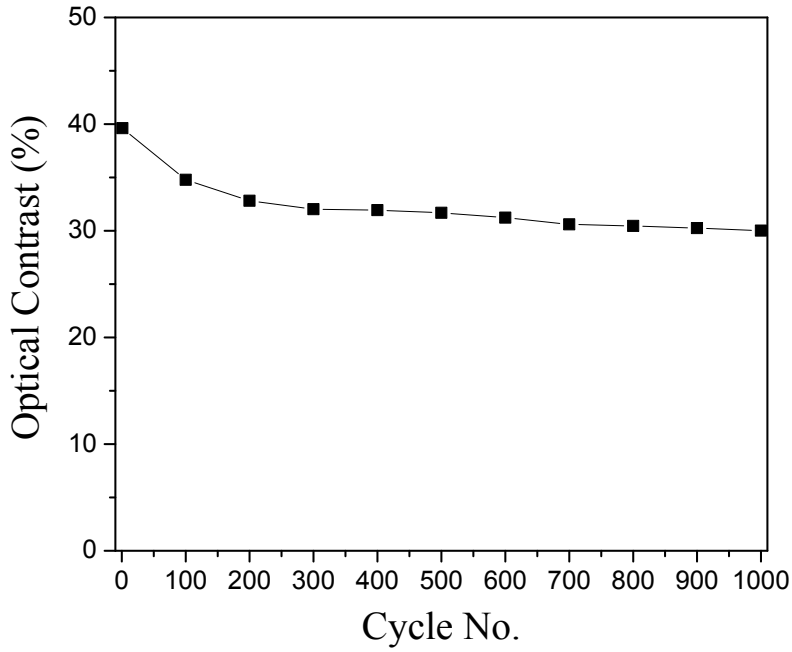
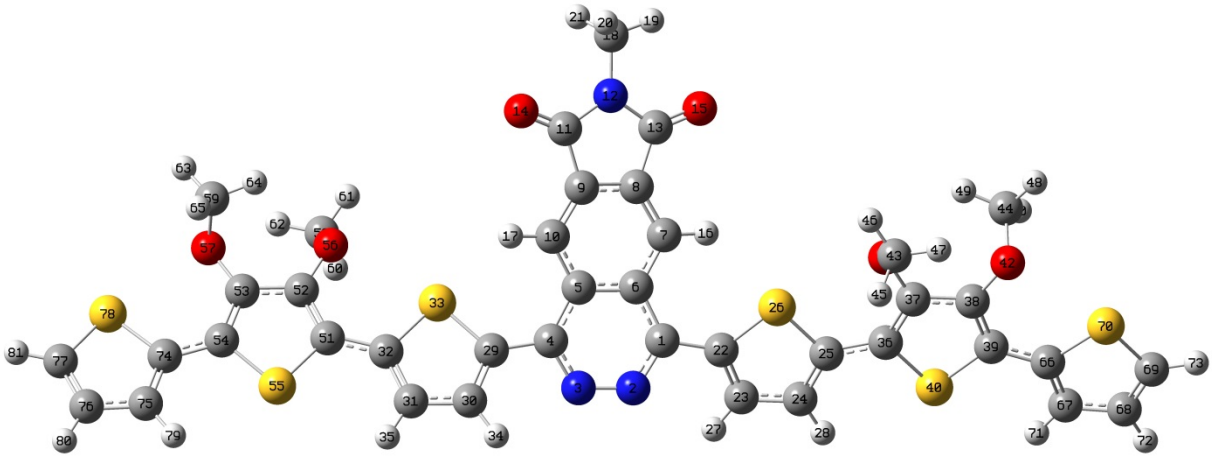


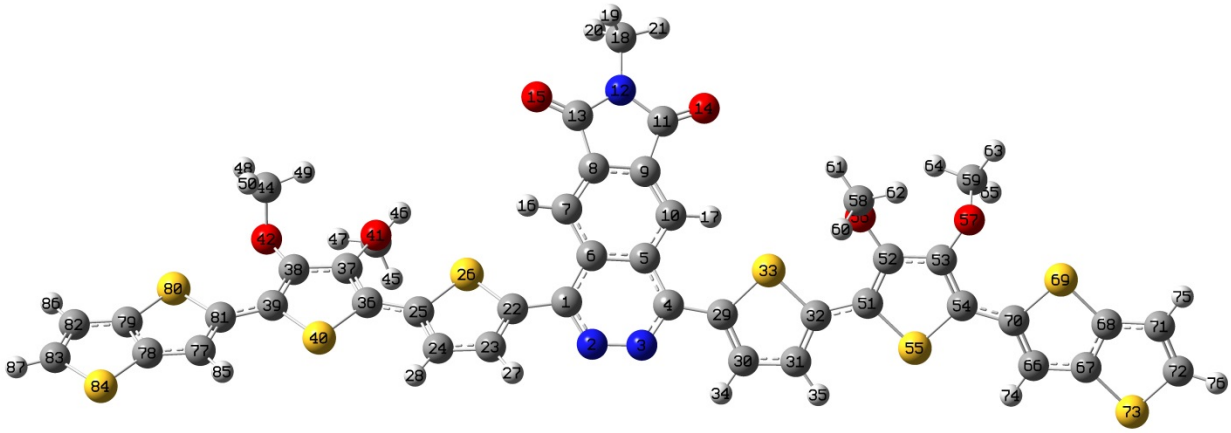
Fig. S5 Stability study of **P2** spin-coated device by monitoring optical contrast as a function of number of cycles between + 1.6 and -1.6 V with a switching time of 15 s.

4. TD-DFT calculations details



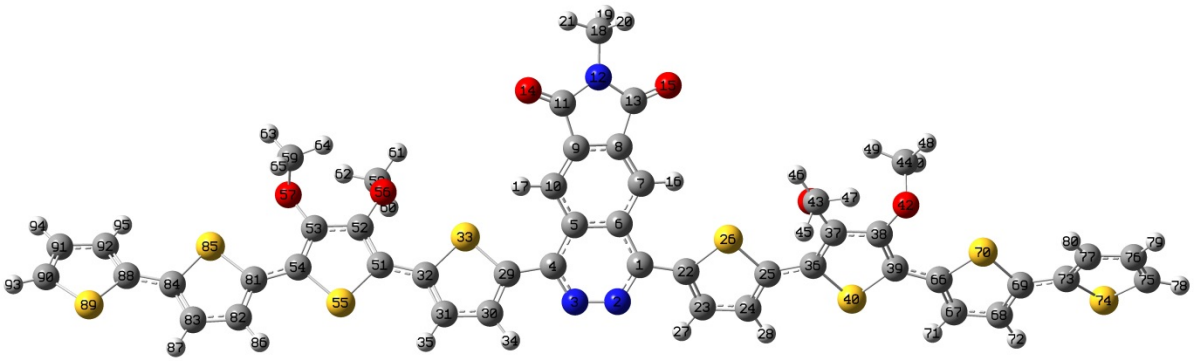
D(2,1,22,23)	24.5197	D(3,4,29,30)	24.3949	D(24,25,36,40)	3.0877
D(6,1,22,26)	30.8908	D(5,4,29,33)	30.7244	D(26,25,36,37)	4.5267
D(31,32,51,55)	2.9535	D(38,39,66,70)	6.4649	D(53,54,74,78)	6.4224
D(33,32,51,52)	4.3784	D(40,39,66,67)	5.4345	D(55,54,74,75)	5.4012

Fig. S6 Torsional angles of optimized geometry of **M1** monomer.



D(2,1,22,23)	24.6695	D(3,4,29,30)	24.9355	D(24,25,36,40)	3.3798
D(6,1,22,26)	30.9981	D(5,4,29,33)	31.5385	D(26,25,36,37)	4.8700
D(31,32,51,55)	3.7125	D(38,39,81,80)	6.5542	D(53,54,70,69)	6.7923
D(33,32,51,52)	5.2745	D(40,39,81,77)	5.4942	D(55,54,70,66)	5.6929

Fig. S7 Torsional angles of optimized geometry of **M2** monomer.



D(2,1,22,23)	24.3403	D(3,4,29,30)	24.3757	D(24,25,36,40)	2.9858
D(6,1,22,26)	30.7083	D(5,4,29,33)	30.6459	D(26,25,36,37)	4.4106
D(31,32,51,55)	3.0517	D(38,39,66,70)	6.0886	D(53,54,81,85)	6.0562
D(33,32,51,52)	4.4650	D(40,39,66,67)	5.1324	D(55,54,81,82)	5.1028
D(68,69,73,74)	17.5027	D(83,84,88,89)	17.6000		
D(70,69,73,77)	17.5344	D(85,84,88,92)	17.6259		

Fig. S8 Torsional angles of optimized geometry of **M3** monomer.

5. NMR spectra of all new compounds

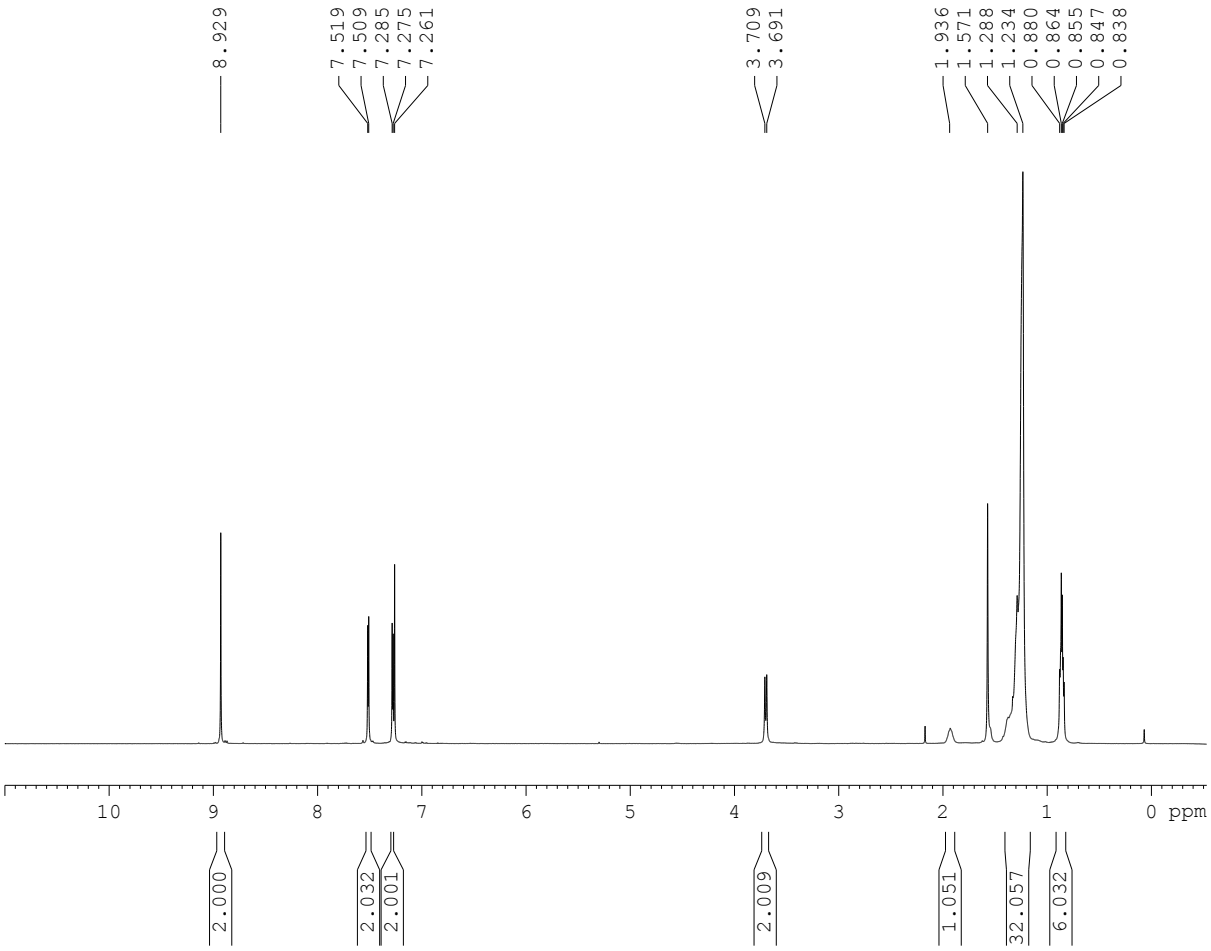


Fig. S9 ^{1}H NMR spectrum of compound **3** ($CDCl_3$, room temperature).

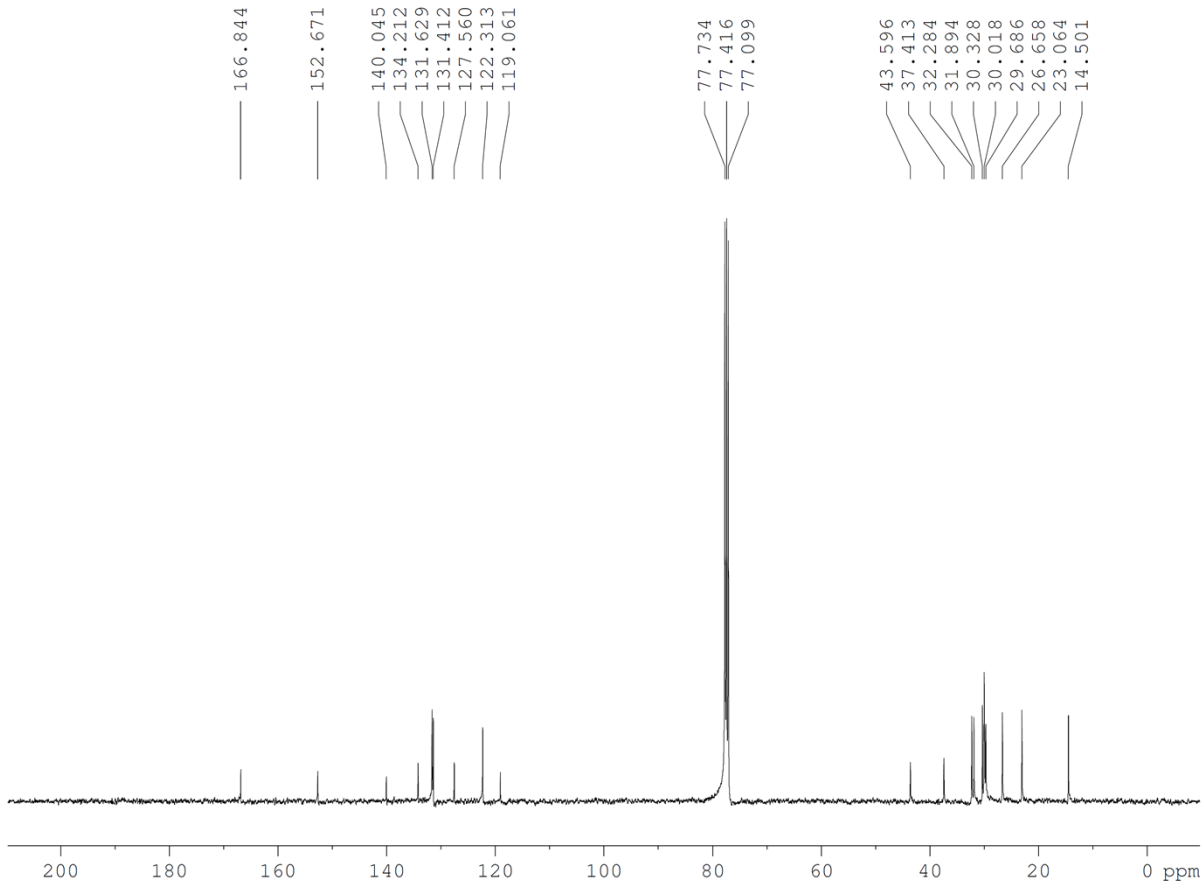


Fig. S10 ^{13}C NMR spectrum of compound **3** ($CDCl_3$, room temperature).

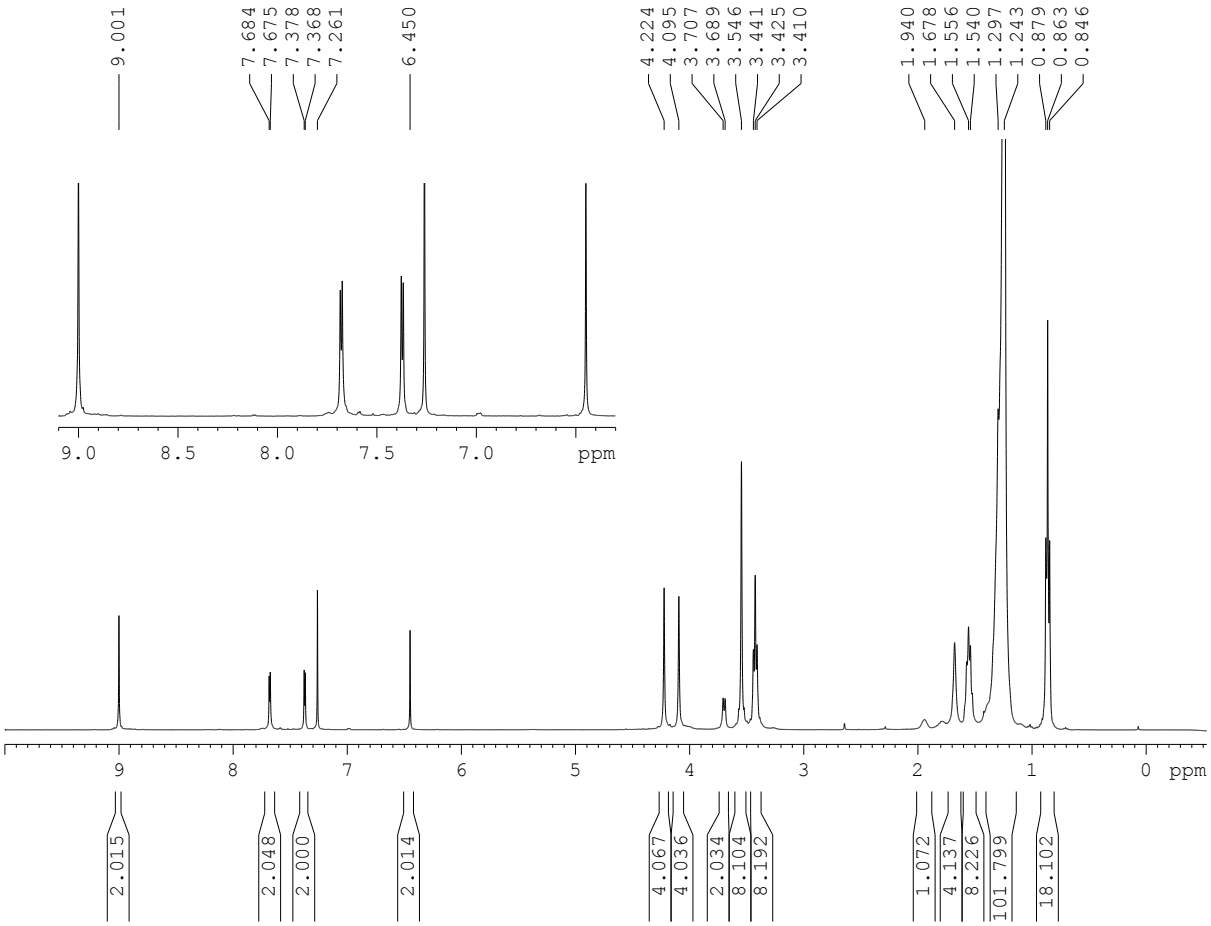


Fig. S11 ^{1}H NMR spectrum of compound **4** ($CDCl_3$, room temperature).

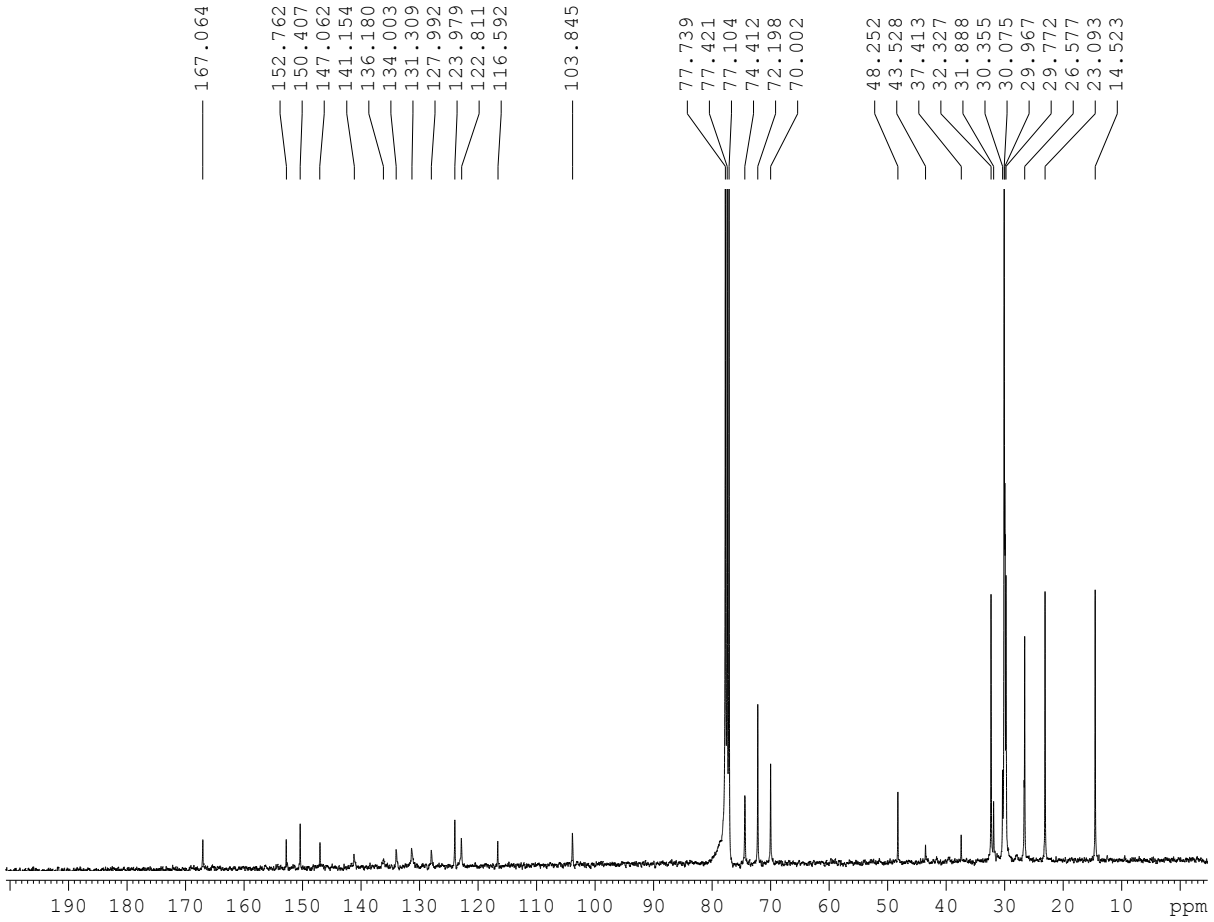


Fig. S12 ^{13}C NMR spectrum of compound **4** ($CDCl_3$, room temperature).

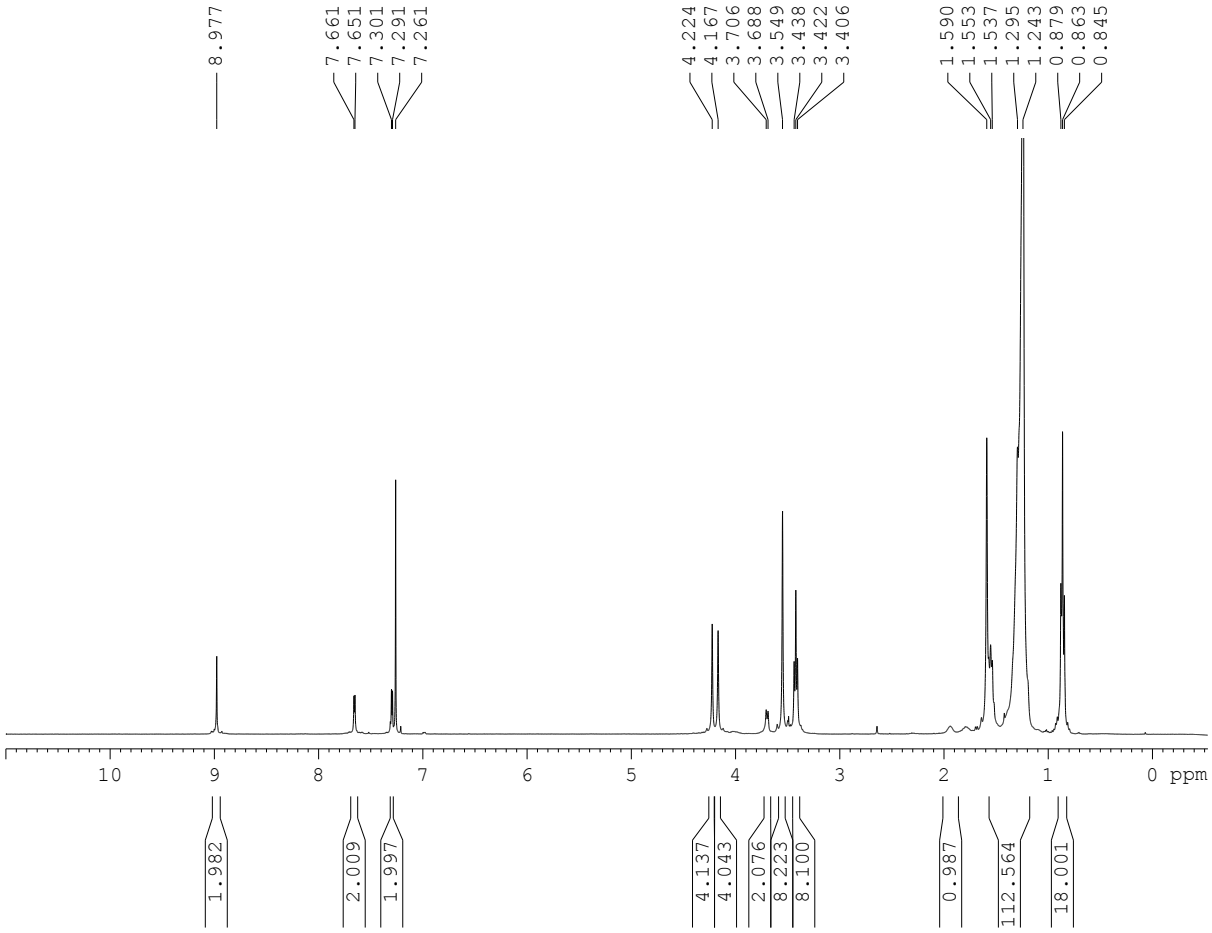


Fig. S13 ^{1}H NMR spectrum of compound **5** ($CDCl_3$, room temperature).

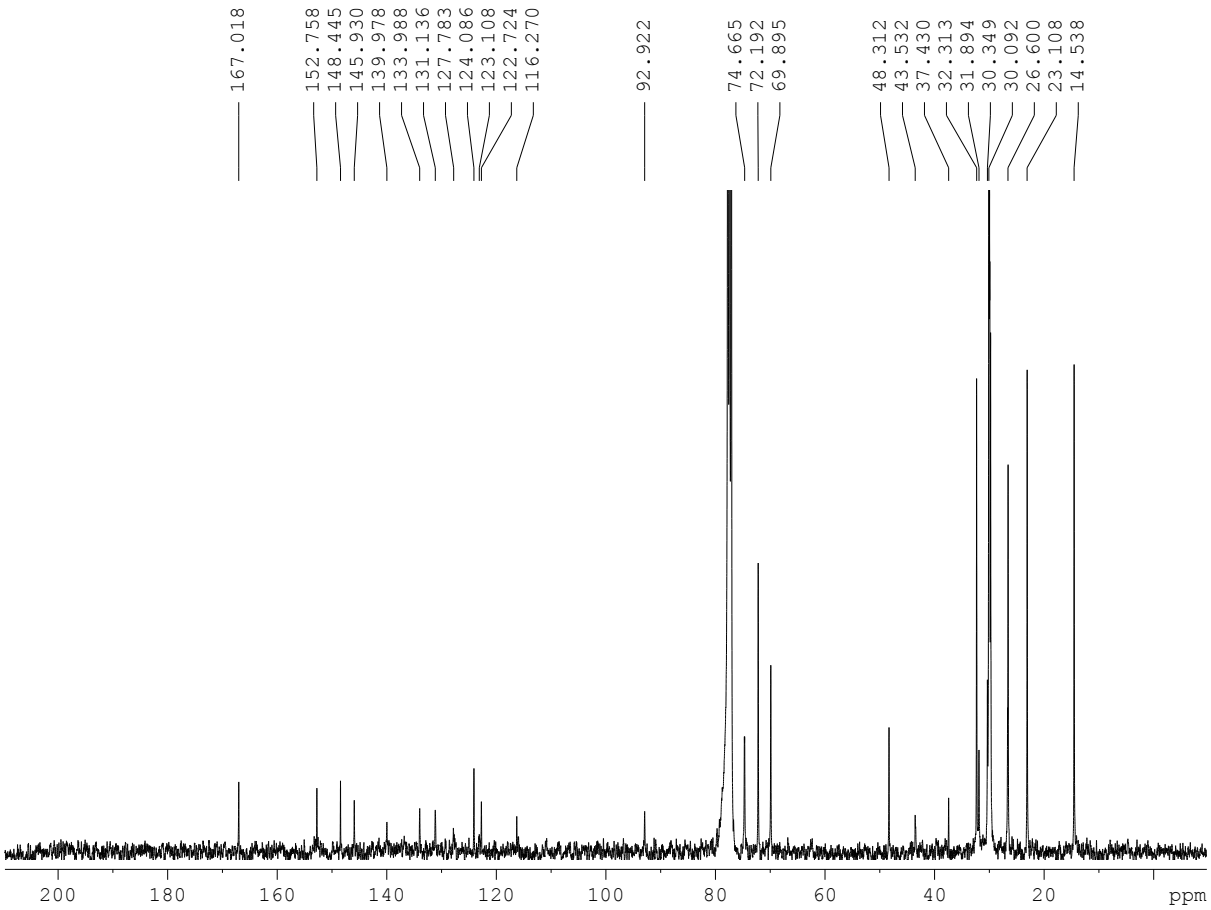


Fig. S14 ^{13}C NMR spectrum of compound **5** ($CDCl_3$, room temperature).

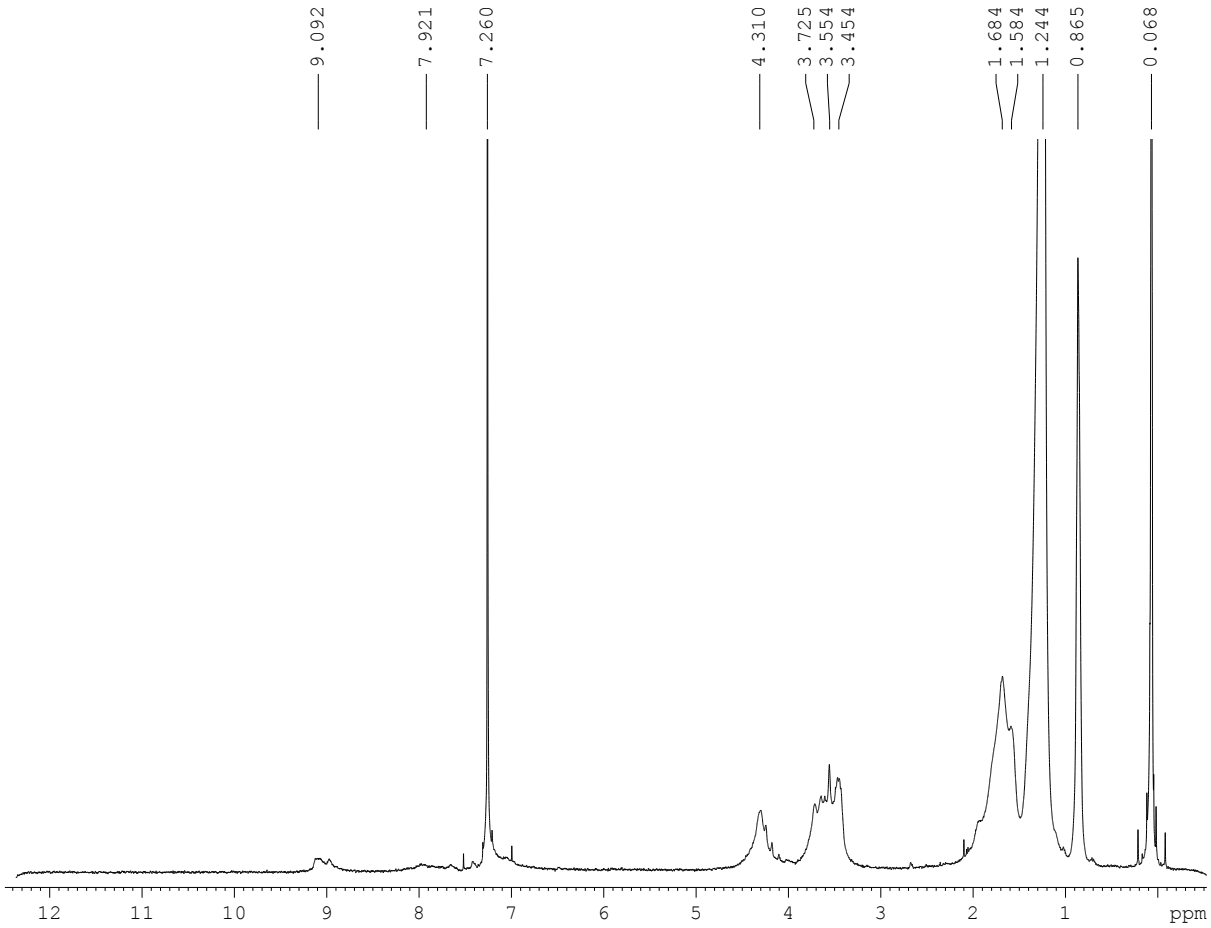


Fig. S15 ^{1}H NMR spectrum of compound **P1** ($CDCl_3$, room temperature).

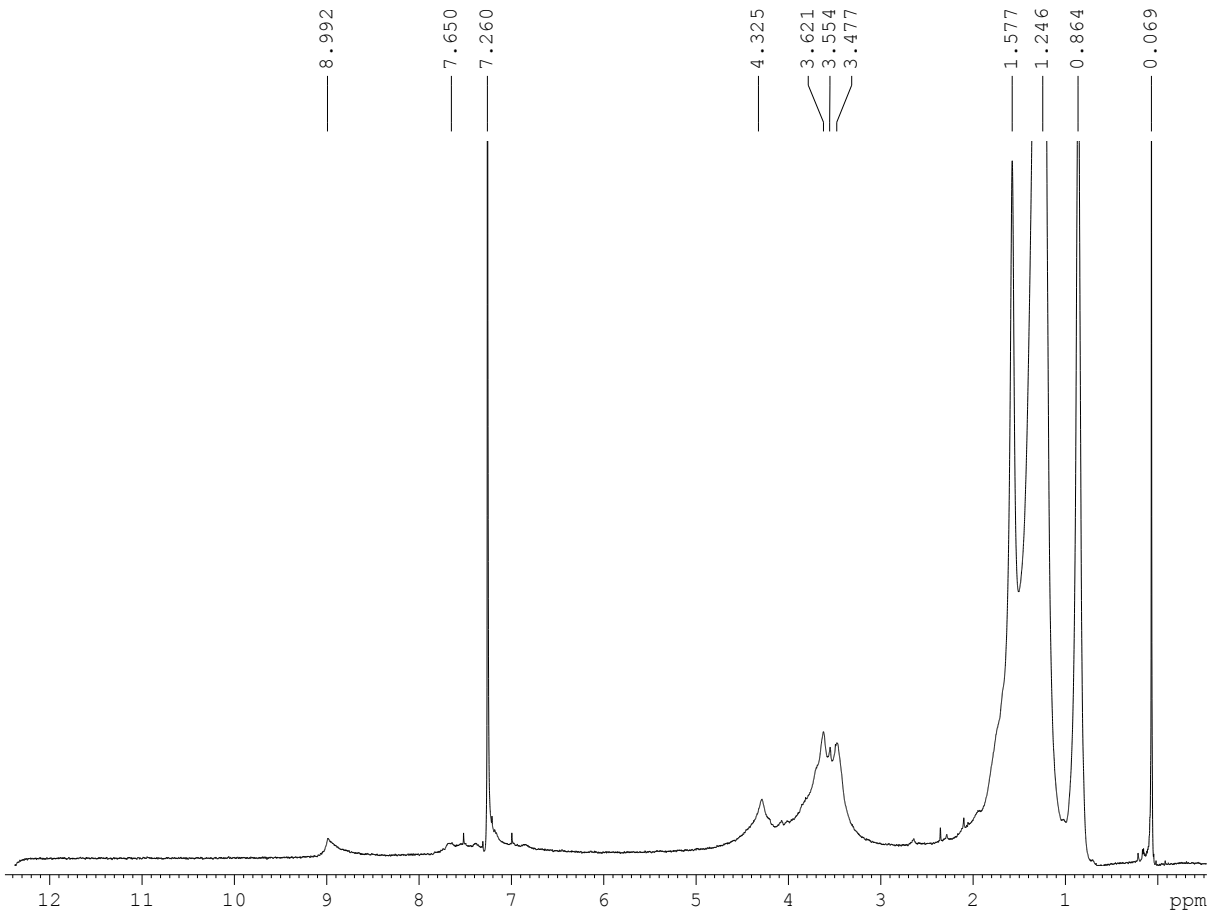


Fig. S16 ^{1}H NMR spectrum of compound **P2** ($CDCl_3$, room temperature).

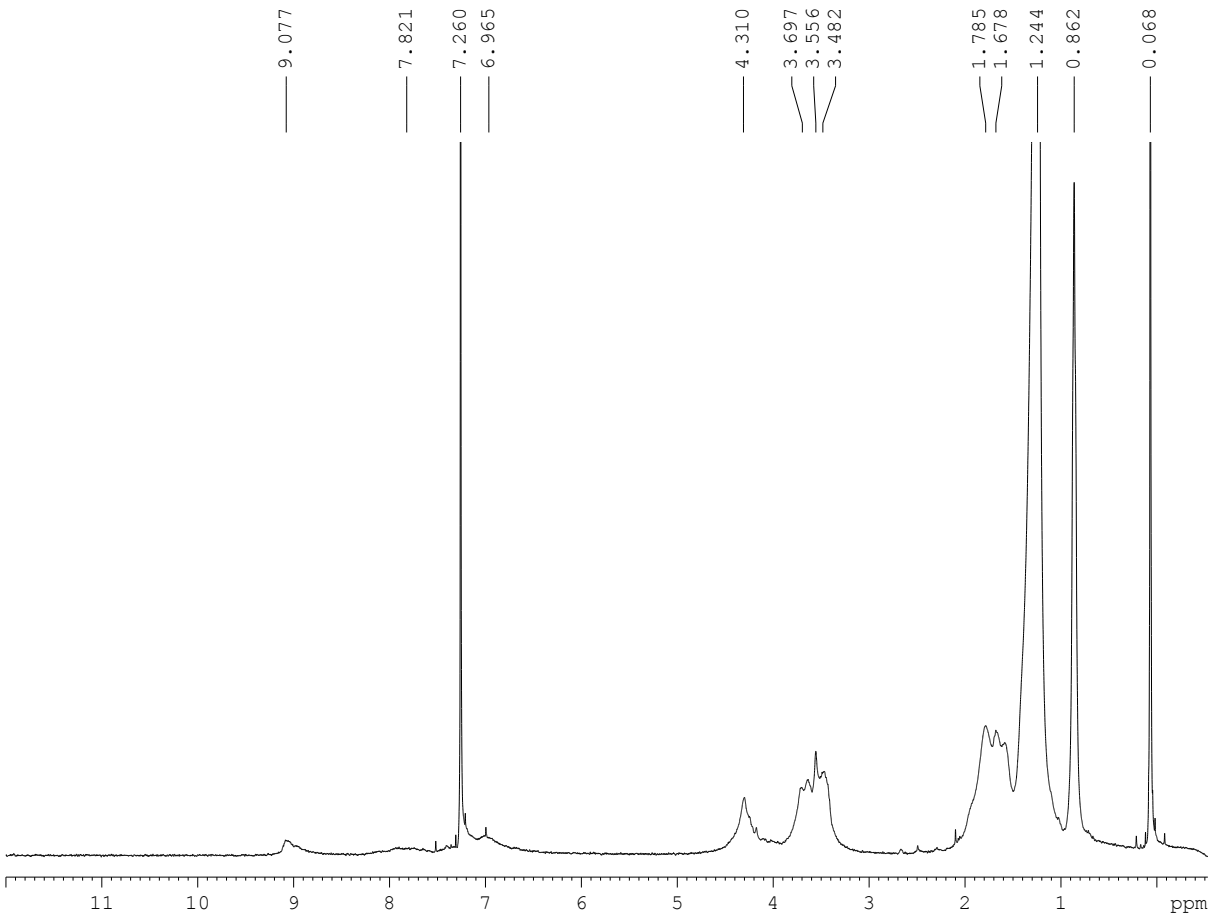


Fig. S17 ^{1}H NMR spectrum of compound **P3** ($CDCl_3$, room temperature).