

Supporting Information

Influence of the regioregularity on the chiral supramolecular organization of poly(3- alkylsulfanylthiophene)s.

Helmuth Peeters, Pauline Couturon, Steven Vandeleene, David Moerman, Philippe Leclère,

Roberto Lazzaroni, Inge De Cat, Steven De Feyter and Guy Koeckelberghs

Table of contents

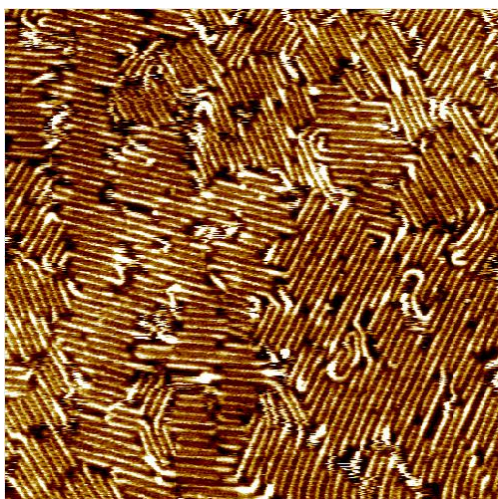
S1.	STM.....	2
S1.1	Fourier transformation	2
S1.2	Histograms	4
S2.	¹ H NMR spectra	5
S2.1	¹ H NMR spectrum of quench 2a' and (2a + 2b) with D ₂ O.....	5
S2.2	¹ H NMR spectrum of P1	6
S2.3	¹ H NMR spectrum of P2	6
S2.4	¹ H NMR spectrum of P3	7
S2.5	¹ H NMR spectrum of P4	7
S2.6	¹ H NMR spectrum of P5	8
S3.	UV-vis spectra.....	9
S3.1	P1 and P2 in CHCl ₃ /CS ₂	9
S4.	Solvatochromism experiment of P1-5.....	10
S4.1	Deconvolution of UV-vis spectra of P1-P5	12
S5.	Emission spectroscopy of P1-P5	13
S5.1	Emission spectroscopy of P1-P5 in CHCl ₃	13
S5.2	Emission spectroscopy of P1 in CHCl ₃ /CS ₂ (8/2)	13
S6.	IR spectra of P1-P5	14

S1. STM

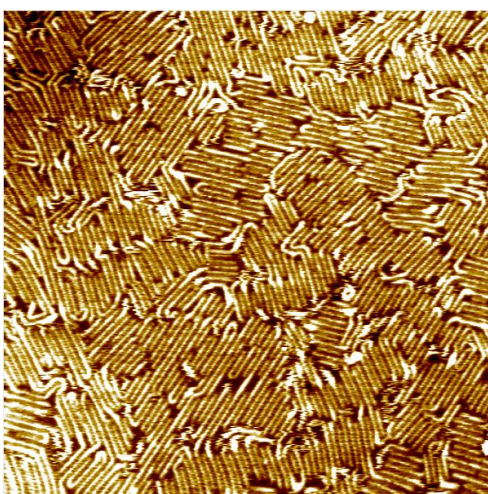
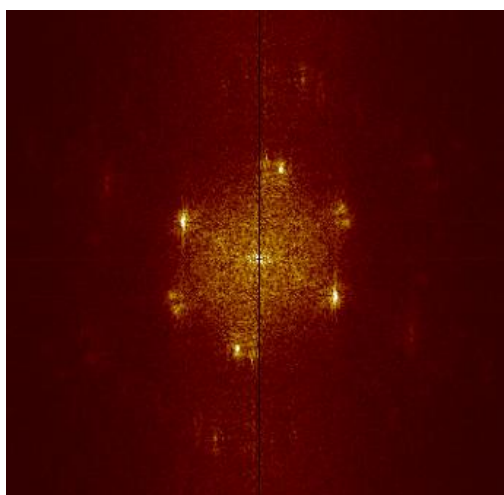
S1.1 *Fourier transformation*

A

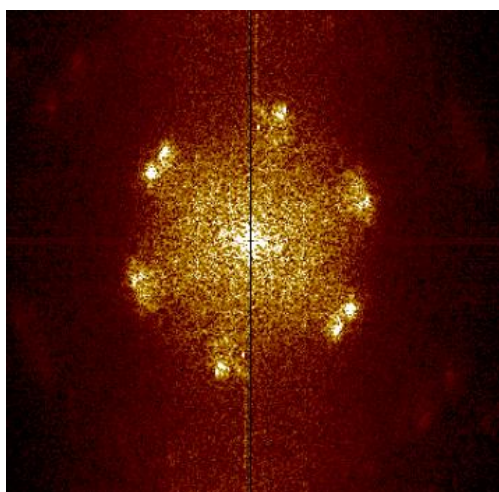
Fourier Analysis



Size: $97.2 \times 97.2 \text{ nm}^2$
 $I_{\text{set}}=127\text{pA}$, $V_{\text{set}}=-860\text{mV}$

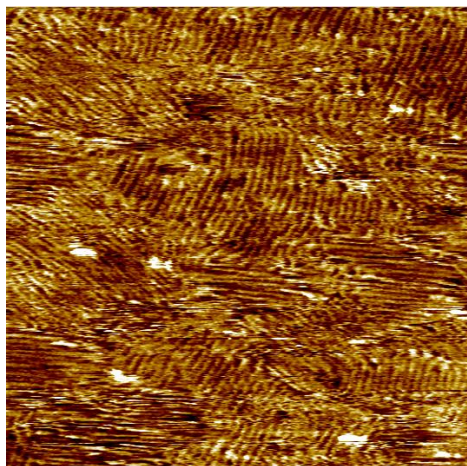


Size: $119 \times 119 \text{ nm}^2$
 $I_{\text{set}}=127\text{pA}$, $V_{\text{set}}=-860\text{mV}$

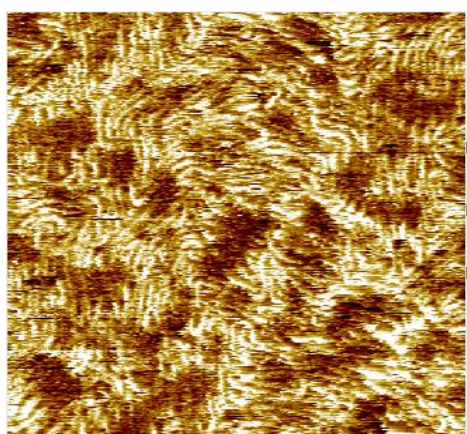
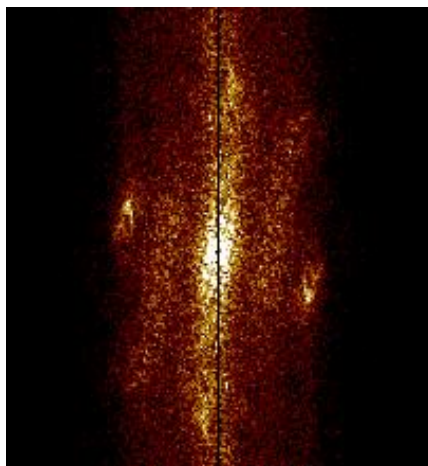


B

Fourier Analysis



Size: $96.4 \times 96.4 \text{ nm}^2$
 $I_{\text{set}}=189\text{pA}$, $V_{\text{set}}=-680\text{mV}$



Size: $104 \times 104 \text{ nm}^2$
 $I_{\text{set}}=127\text{pA}$, $V_{\text{set}}=-860\text{mV}$

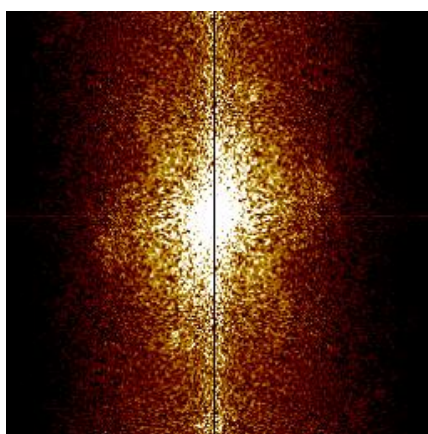
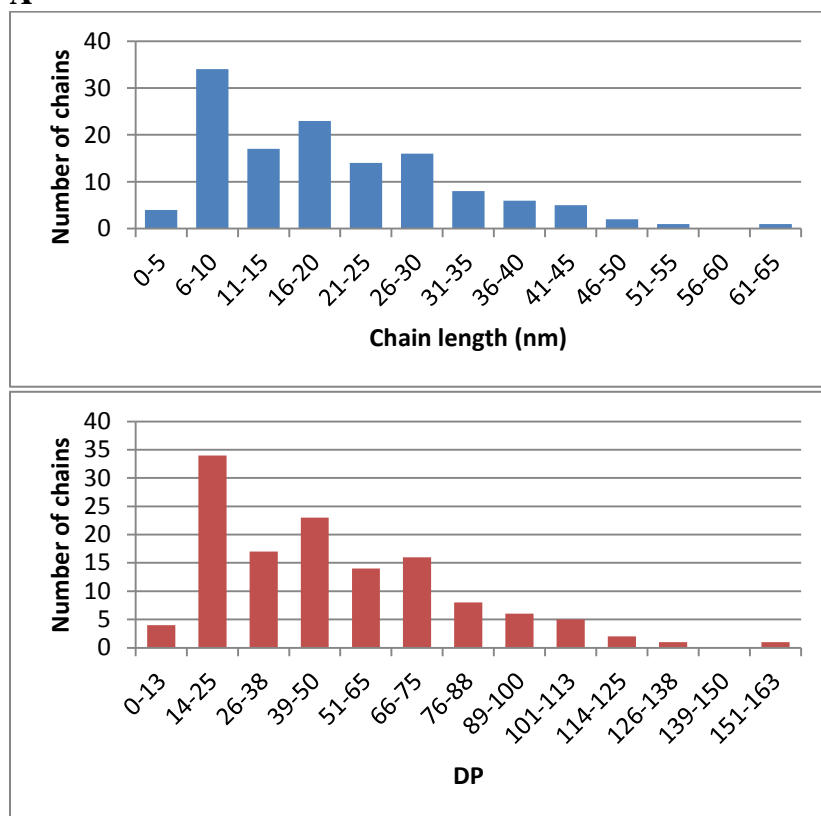


Figure S 1. STM images and the Fourier transformation of the regio-regular P3AST (A) and regio-irregular P3AST (B) at the 1,2,4-TCB/graphite interface. The polymers used are the same as described in *Macromolecules*, 2008, 41, 5123-5131.

S1.2 Histograms

A



B

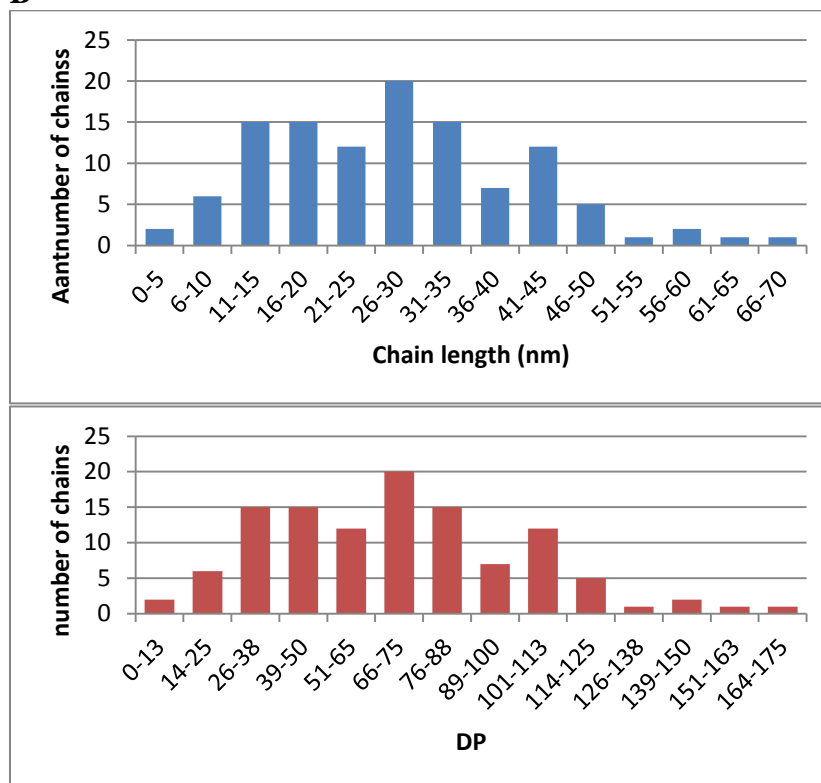


Figure S 2. Histograms showing the distribution of the lengths and DP of self-assembled of the regioregular P3AST (A) and the regio-irregular P3AST (B) chains at the 1,2,4-TCB/graphite interface.

S2. ^1H NMR spectra

S2.1 ^1H NMR spectrum of quench $2a'$ and $(2a + 2b)$ with D_2O

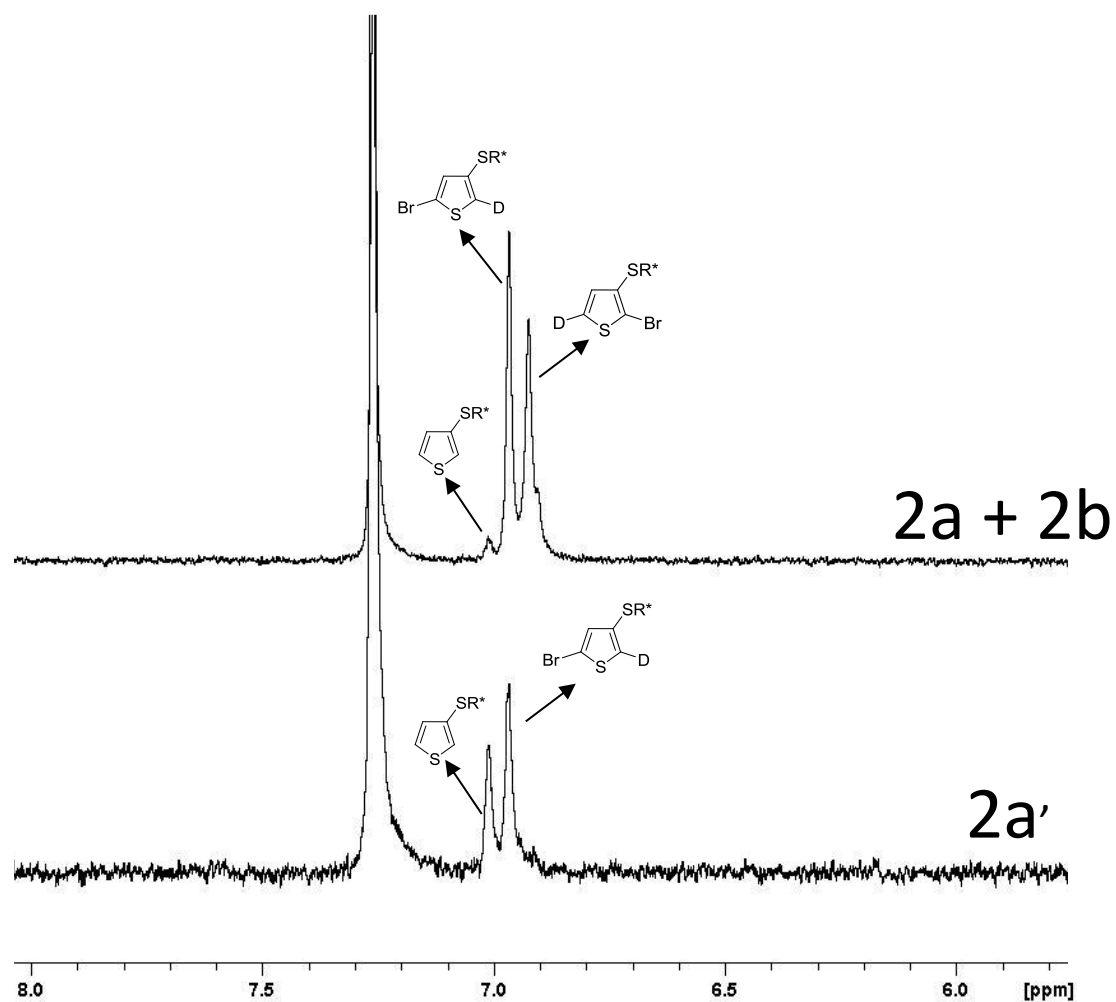
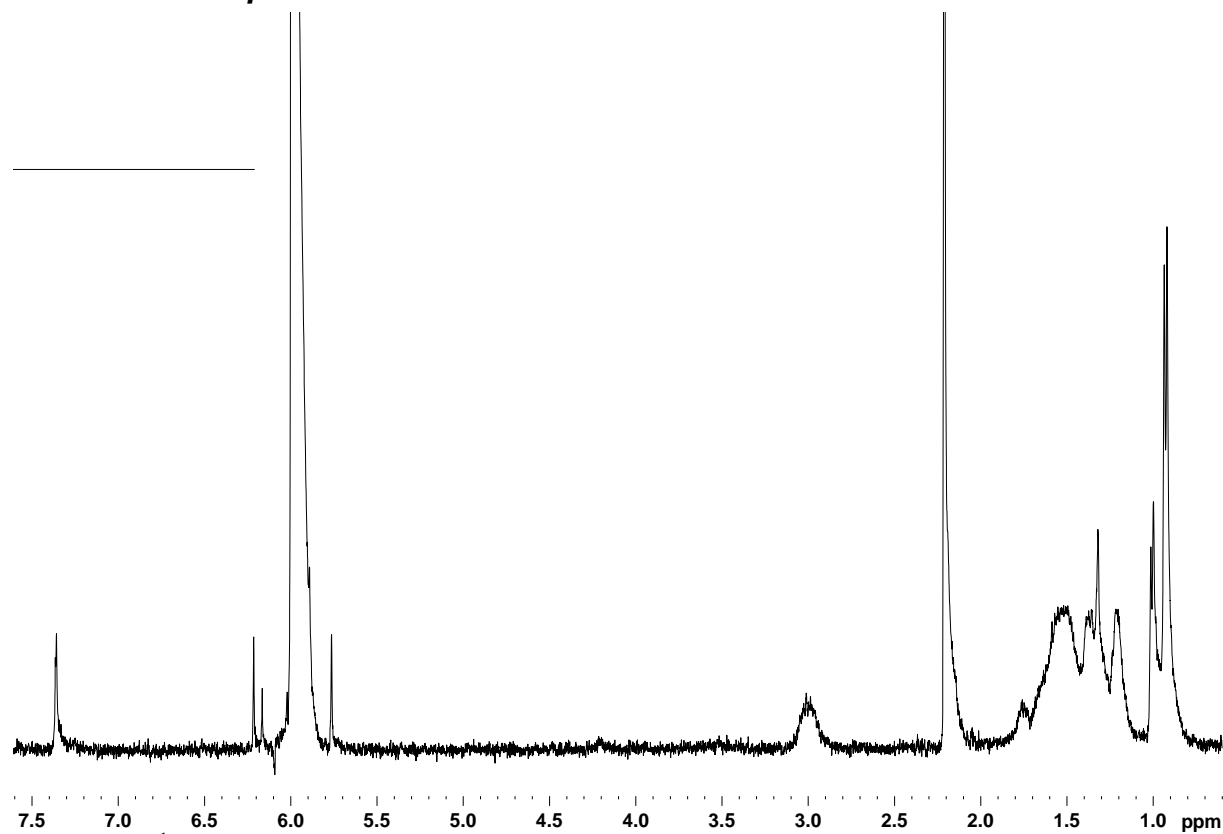
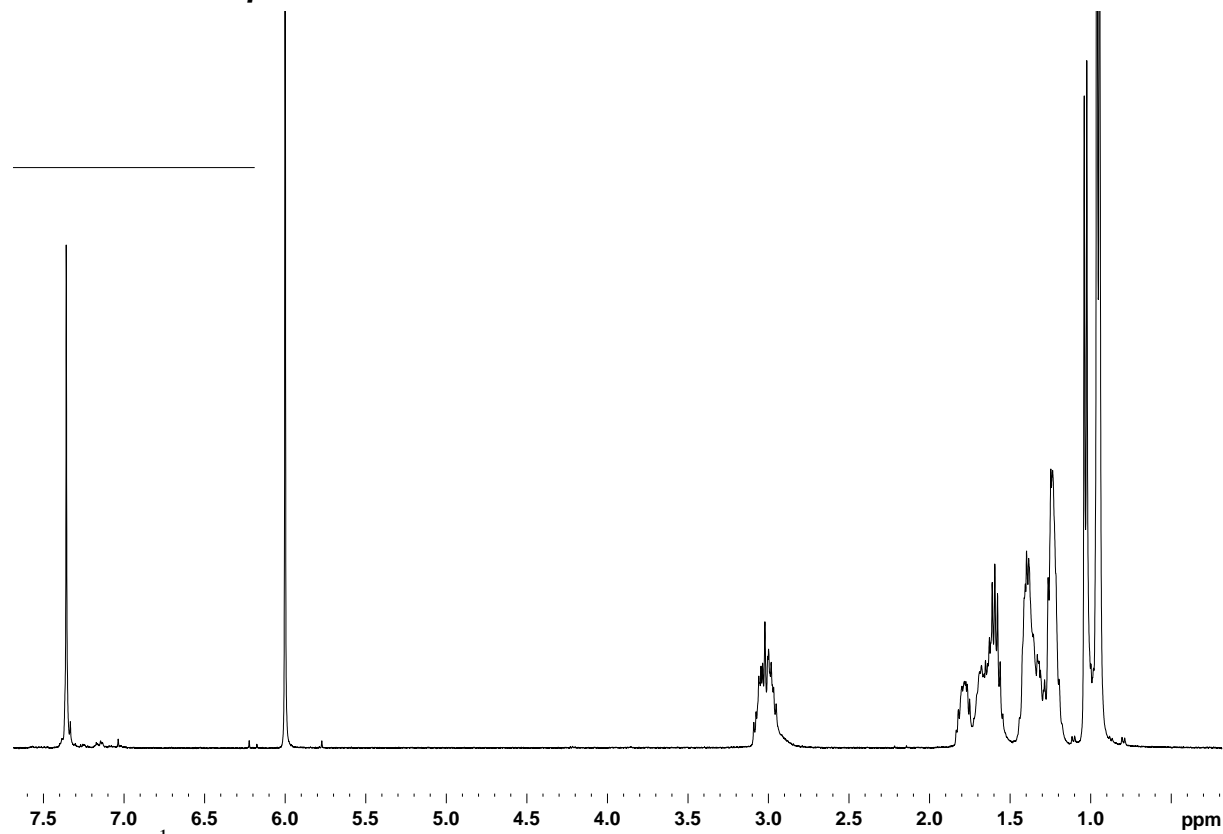


Figure S 3. ^1H NMR (CDCl_3) of the aromatic region of the quench of $2a'$ and $(2a + 2b)$ with D_2O .

S2.2 ^1H NMR spectrum of P1



S2.3 ^1H NMR spectrum of P2



S2.4 ^1H NMR spectrum of P3

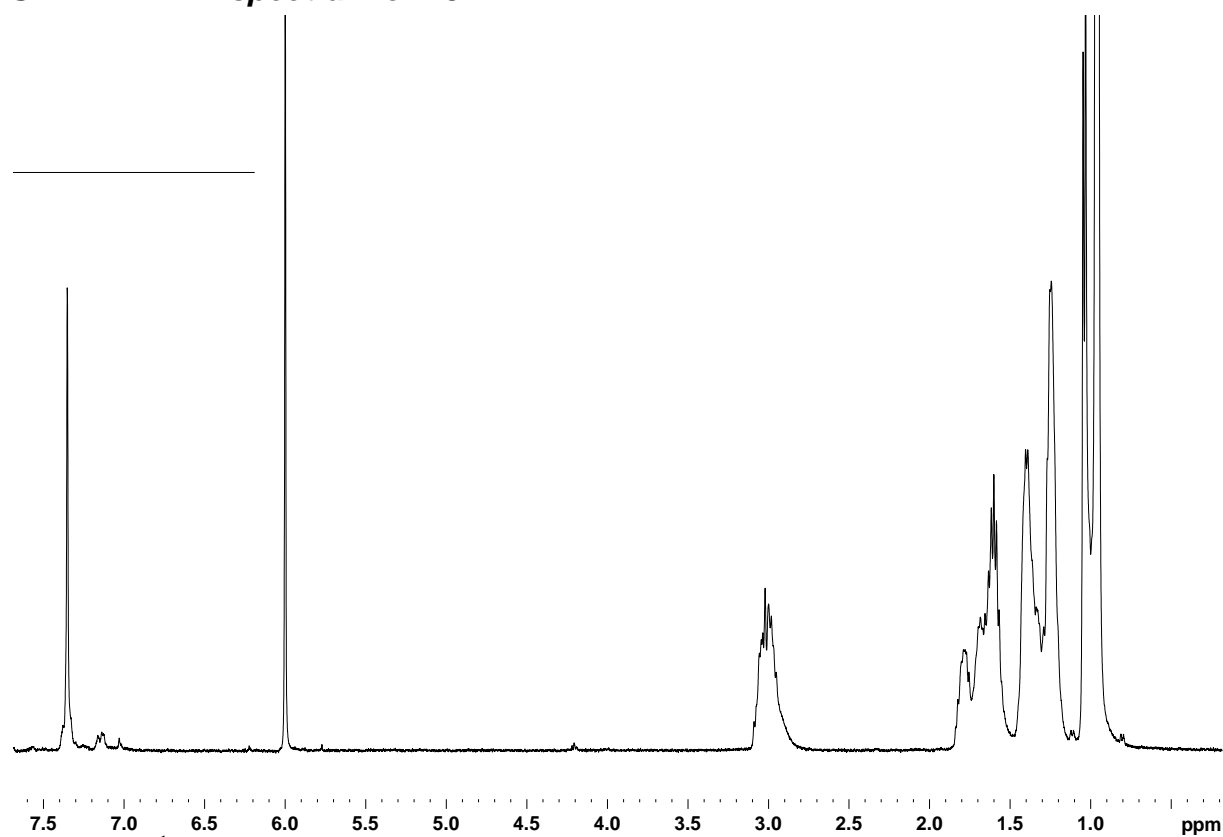


Figure S 6. ^1H NMR ($\text{CS}_2/\text{C}_2\text{D}_2\text{CL}_4$) of P3.

S2.5 ^1H NMR spectrum of P4

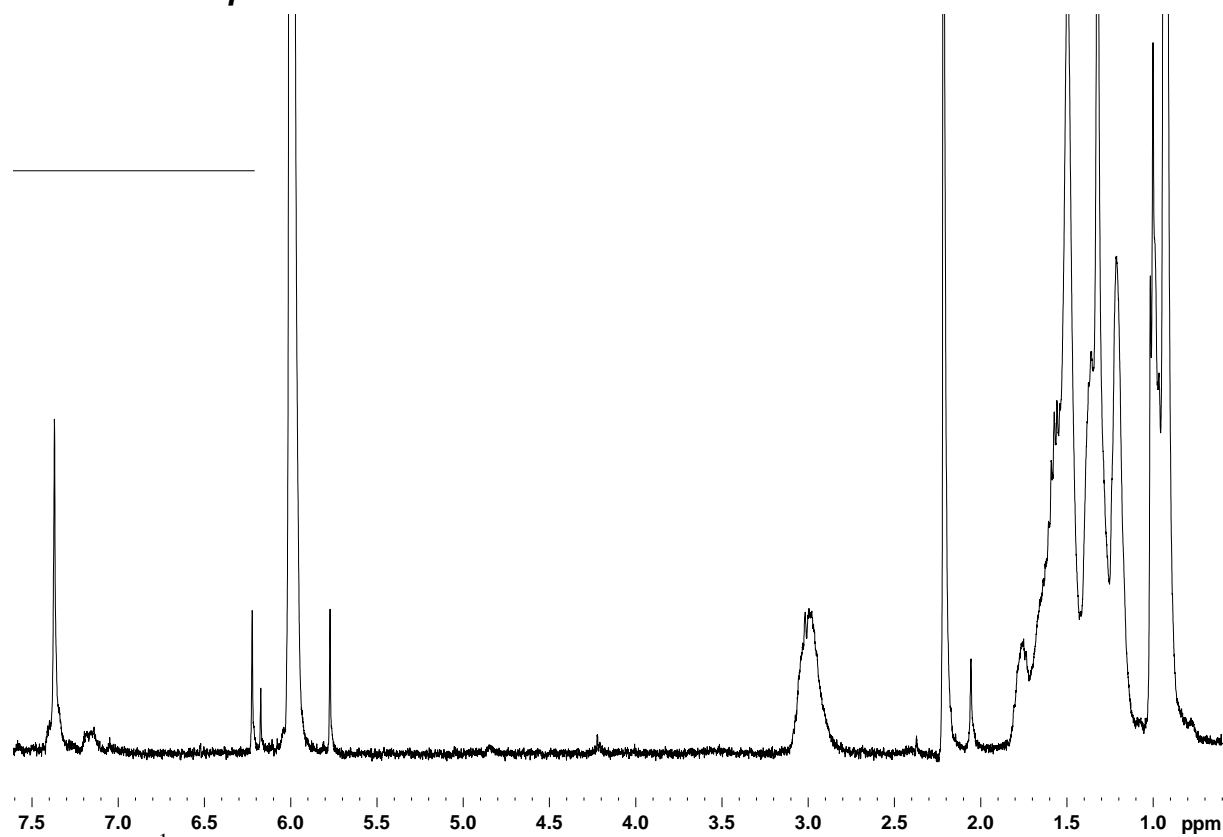


Figure S 7. ^1H NMR ($\text{CS}_2/\text{C}_2\text{D}_2\text{CL}_4$) of P4.

S2.6 ^1H NMR spectrum of P5

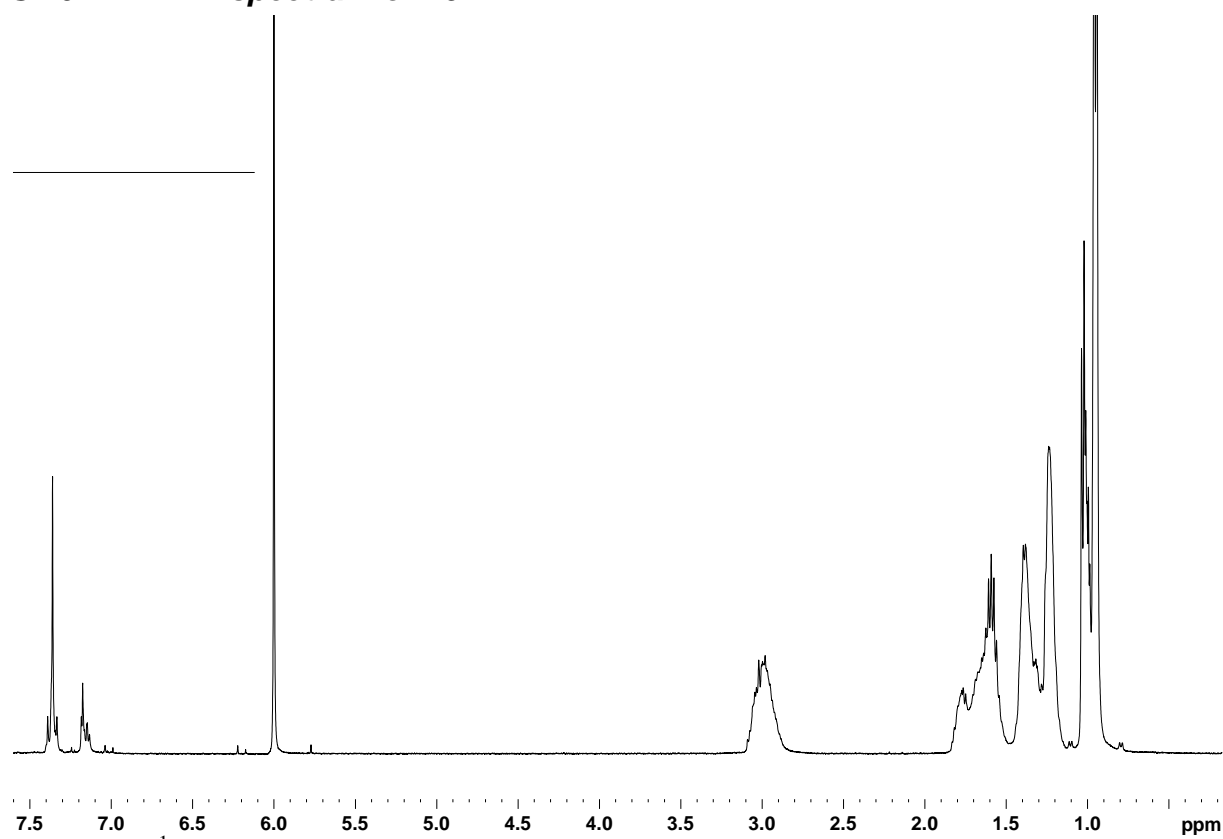


Figure S 8. ^1H NMR ($\text{CS}_2/\text{C}_2\text{D}_2\text{Cl}_4$) of **P5**.

S3. UV-vis spectra

S3.1 P1 and P2 in CHCl₃/CS₂

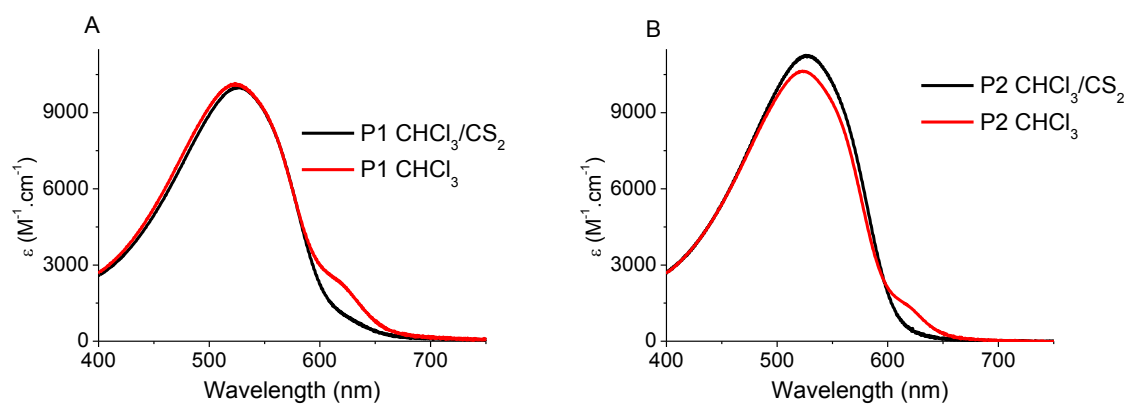


Figure S 9. Complete dissolution of **P1**(A) and **P2**(B) in CHCl₃/CS₂ vs **P1** in CHCl₃.

S4. Solvatochromism experiment of P1-5

S4.1 Solvatochromism

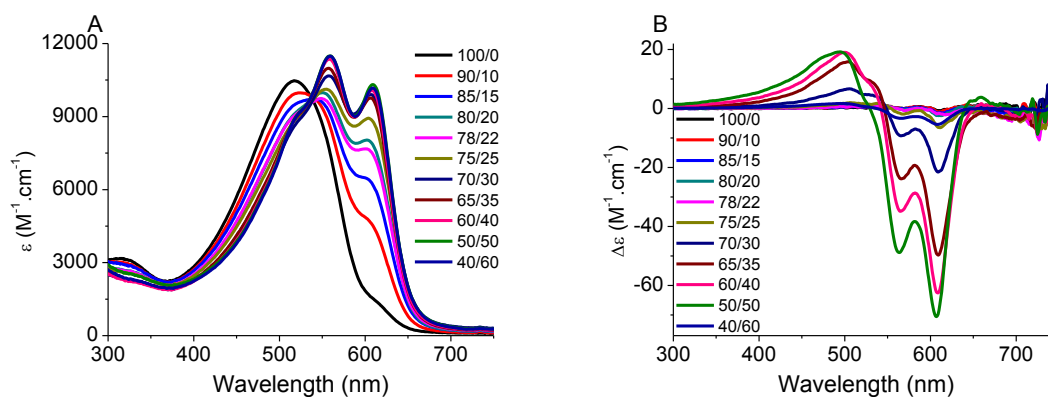


Figure S 10. Solvatochromism experiment of **P1** in $\text{CHCl}_3/\text{MeOH}$ mixtures: A) UV-vis spectra and B) CD spectra.

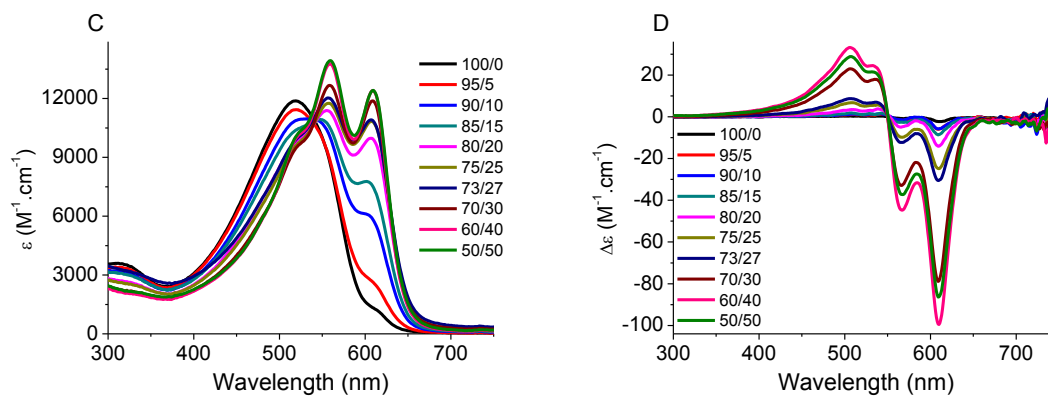


Figure S 11. Solvatochromism experiment of **P2** in $\text{CHCl}_3/\text{MeOH}$ mixtures: C) UV-vis spectra and D) CD spectra.

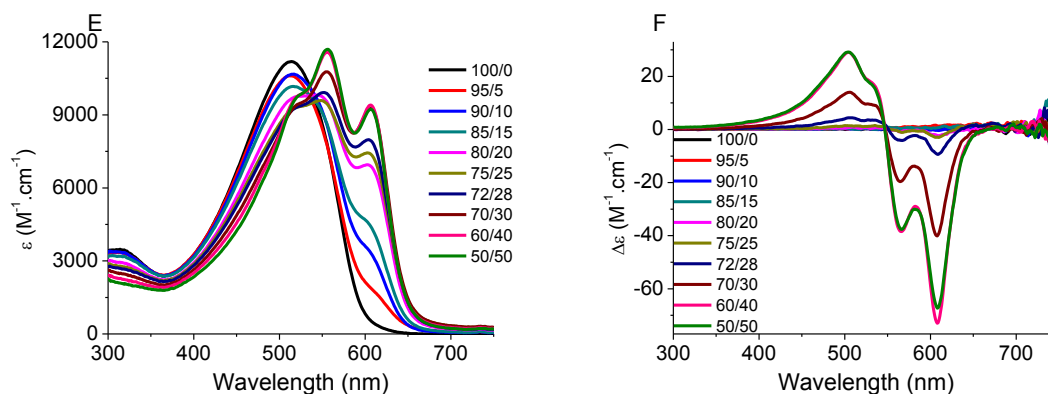


Figure S 12. Solvatochromism experiment of **P3** in $\text{CHCl}_3/\text{MeOH}$ mixtures: E) UV-vis spectra and F) CD spectra.

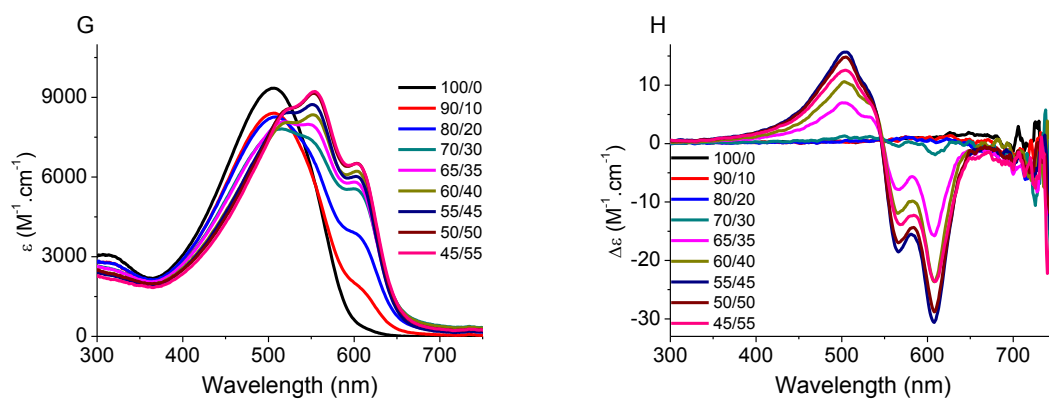


Figure S 13. Solvatochromism experiment of **P4** in CHCl₃/MeOH mixtures: G) UV-vis spectra and H) CD spectra.

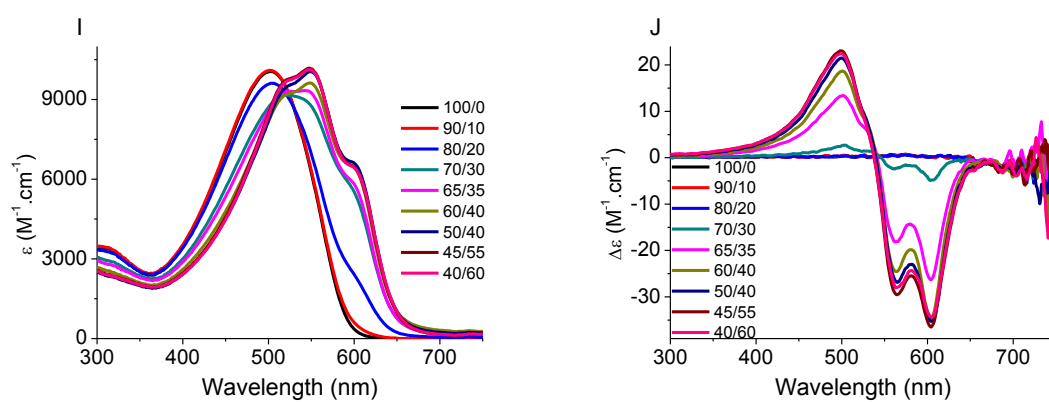


Figure S 14. Solvatochromism experiment of **P5** in CHCl₃/MeOH mixtures: I) UV-vis spectra and J) CD spectra.

S4.2 Deconvolution of UV-vis spectra of P1-P5

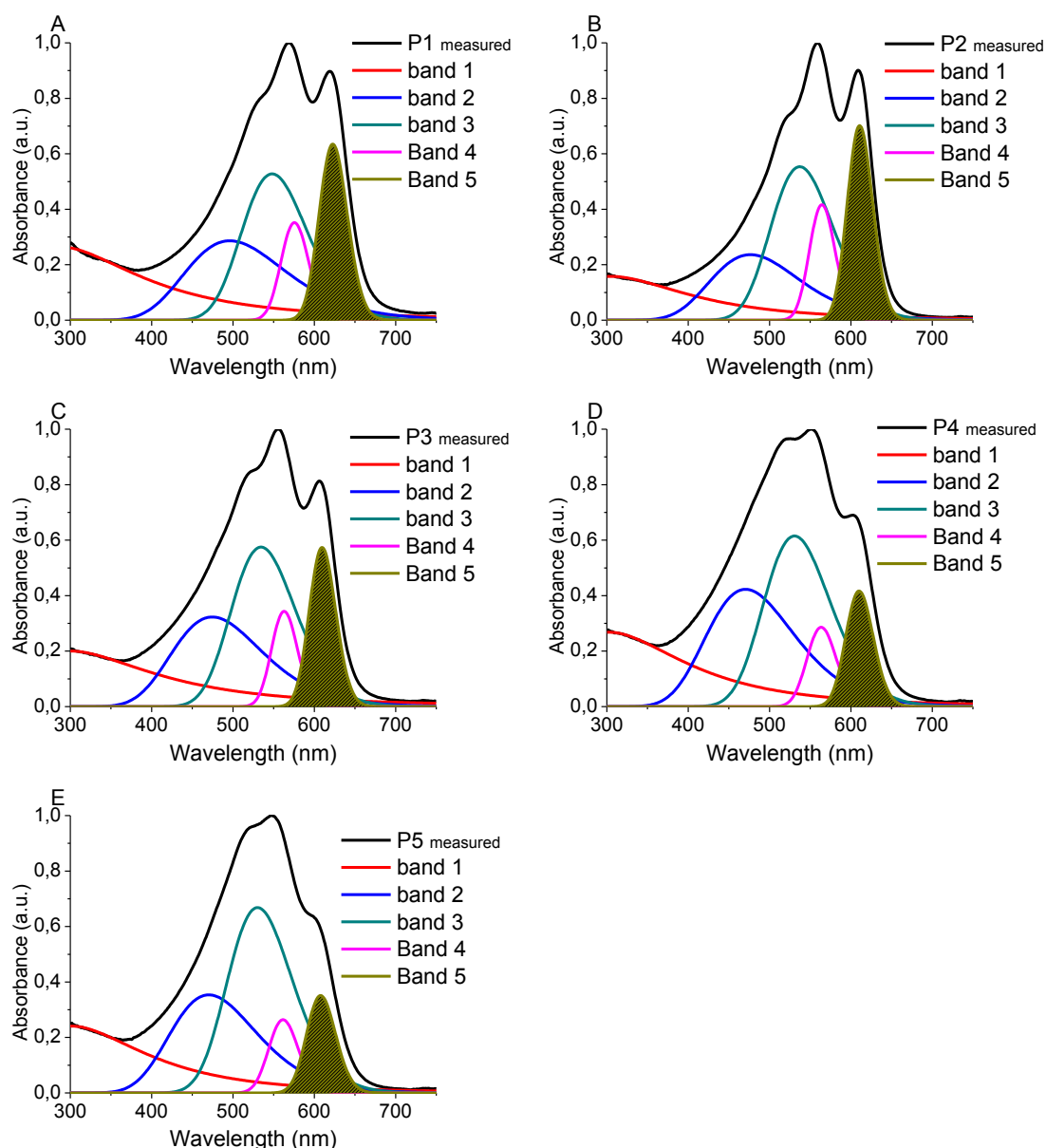


Figure S 15. Deconvolution of UV-vis spectra of P1-P5 in poor solvent mixtures. The band near 610 nm, which probes π interactions, was filled and the relative integration was calculated. A) **P1** CHCl₃/MeOH (50/50); 15.3%, B) **P2** CHCl₃/MeOH (60/40); 17.8%, C) **P3** CHCl₃/MeOH (60/40); 13.5%, D) **P4** CHCl₃/MeOH (55/45); 9.2%, E) **P5** CHCl₃/MeOH (45/55); 8.9%.

S5. Emission spectroscopy of P1-P5

S5.1 Emission spectroscopy of P1-P5 in CHCl_3

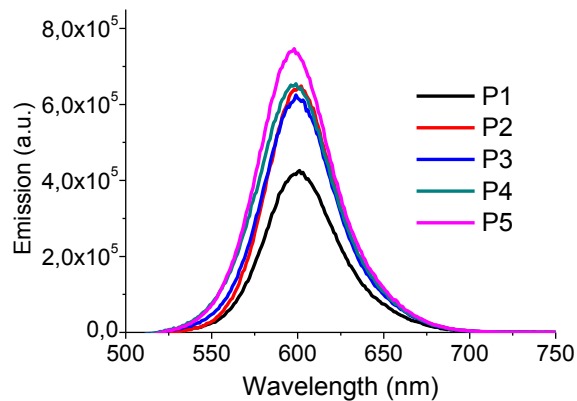


Figure S 16. Emission spectra of **P1-P5** in CHCl_3 excited at 500 nm.

S5.2 Emission spectroscopy of P1 in $\text{CHCl}_3/\text{CS}_2$ (8/2)

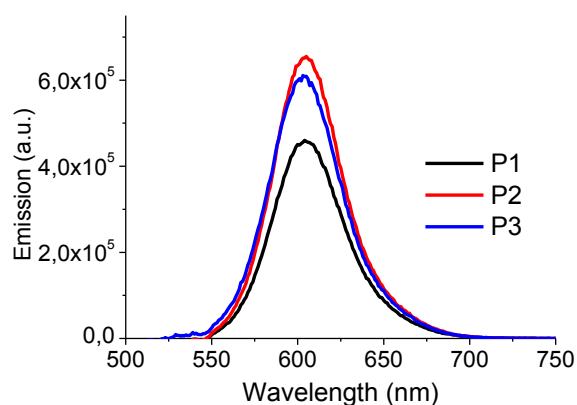


Figure S 17. Emission spectra of **P1-P3** in $\text{CHCl}_3/\text{CS}_2$ (8/2) excited at 500 nm.

S6. IR spectra of P1-P5

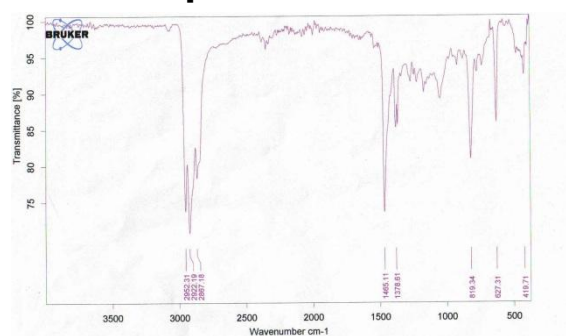


Figure S 18. IR spectrum P1.

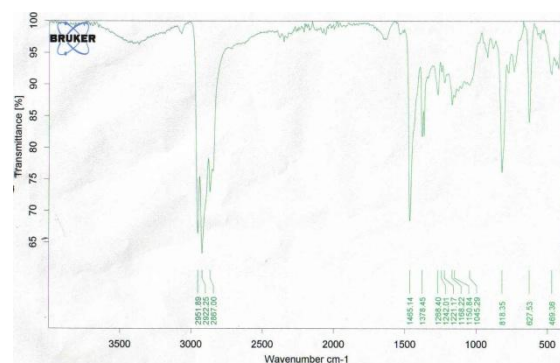


Figure S 22. IR spectrum P1.

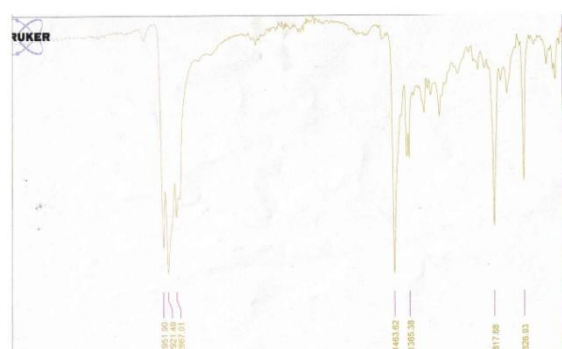


Figure S 19. IR spectrum P2.

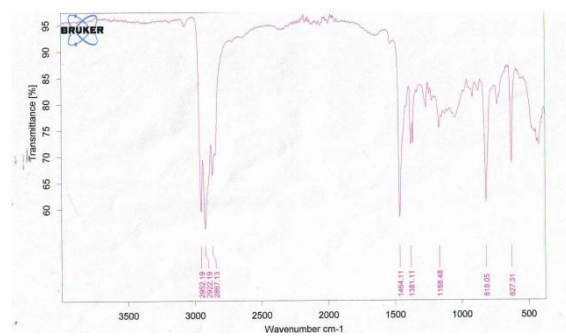


Figure S 20. IR spectrum P3.

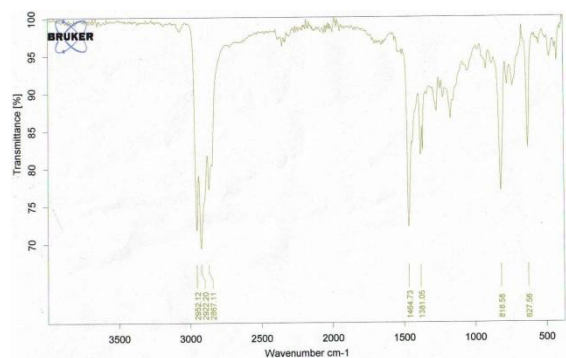


Figure S 21. IR spectrum P3.