Supporting information

Phenyleneethynylene and Thienyleneethynylene-based π-Conjugated Polymers with Imidazolium Units in the Main Chain

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(1) NMR Spectra (×are due to solvent impurities)

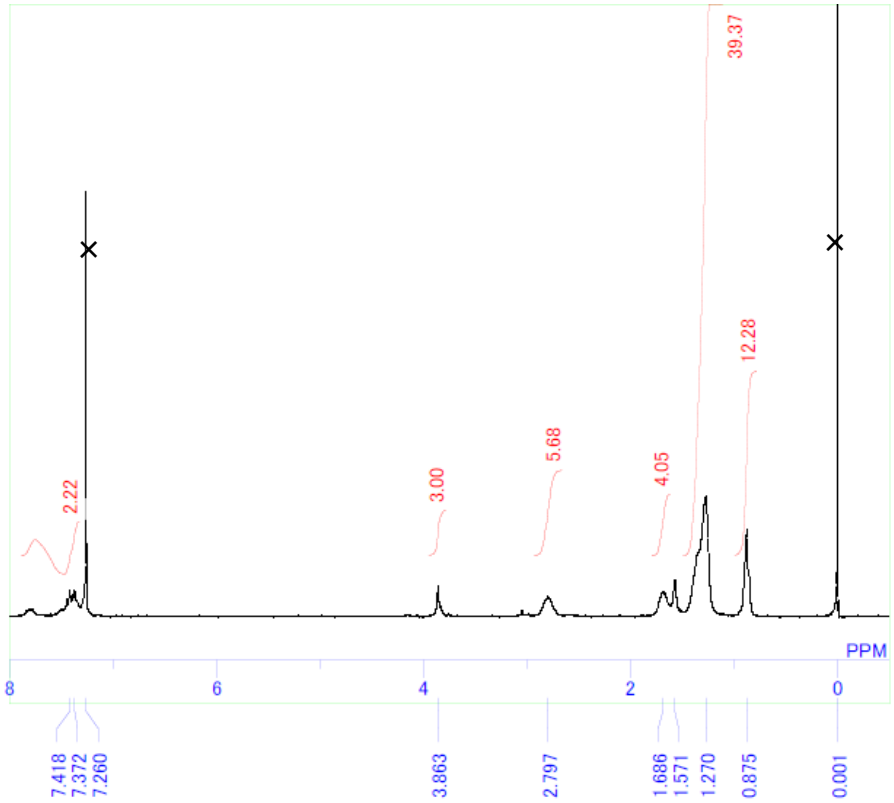


Figure S1. ^{1}H NMR of **P1** in $CDCl_3$

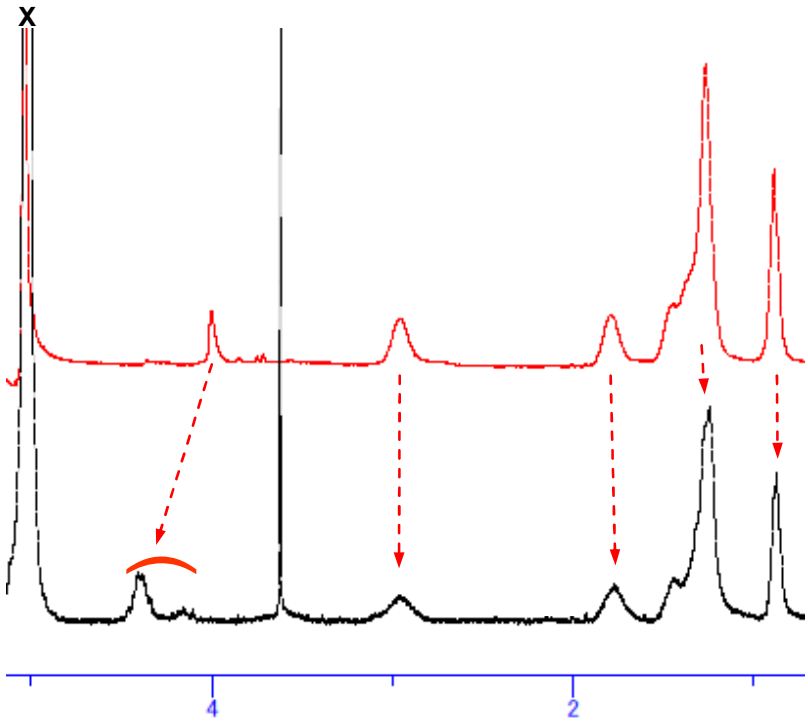


Figure S2. ^{1}H NMR of **P1** (top) and **P2** (bottom) in pyridine-d_5.

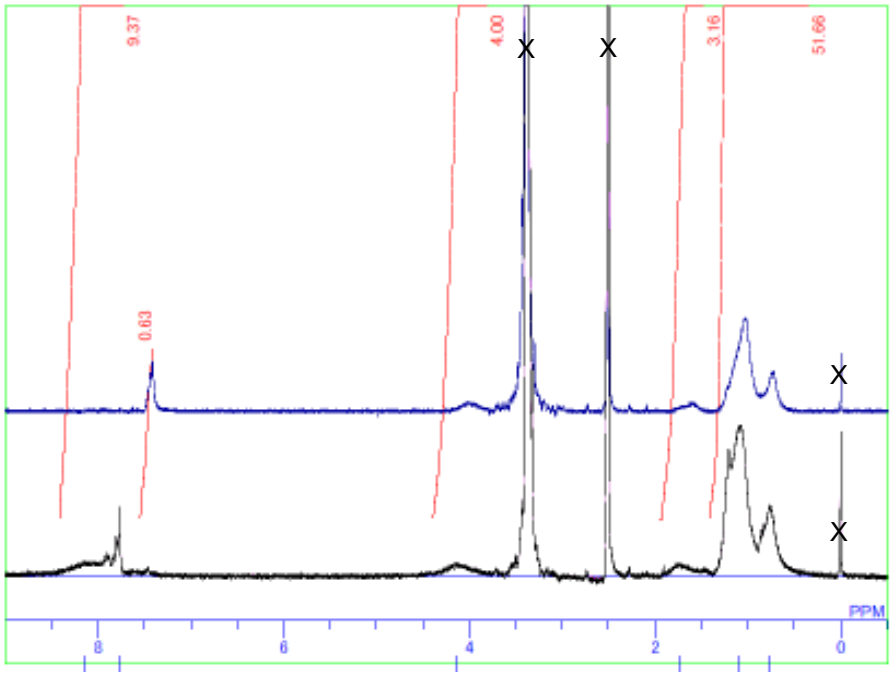


Figure S3. ^{1}H NMR of **P4** (top) and **P5** (bottom) in pyridine-d_5.

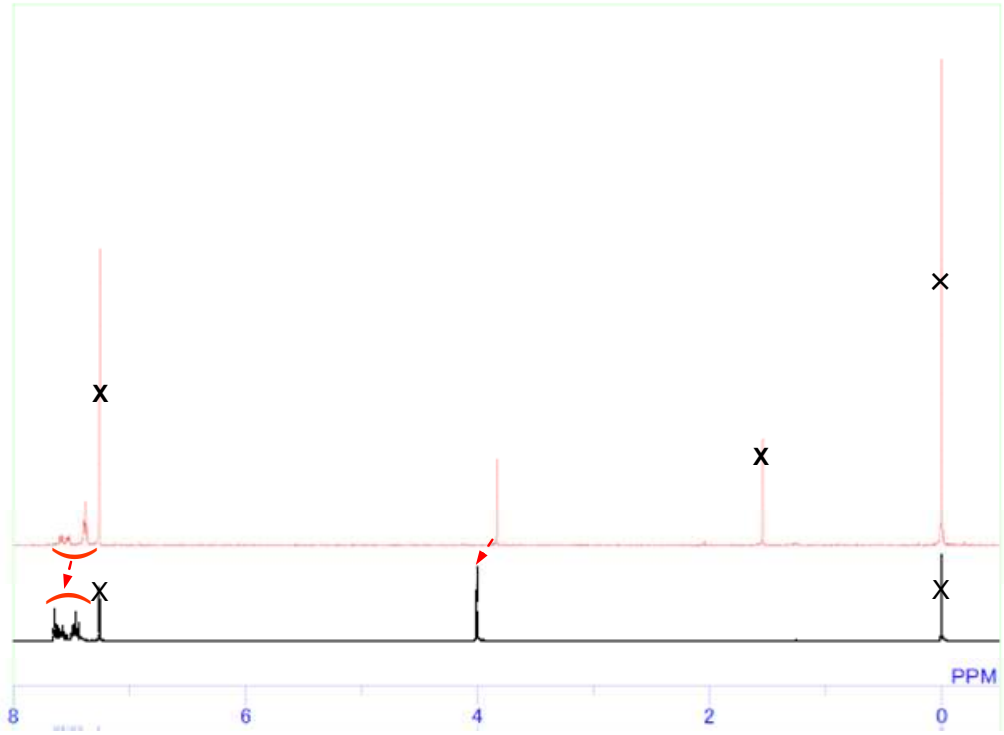


Figure S3. ^{1}H NMR of **M1** adding TFA before (red) and after (black) in $CDCl_3$.

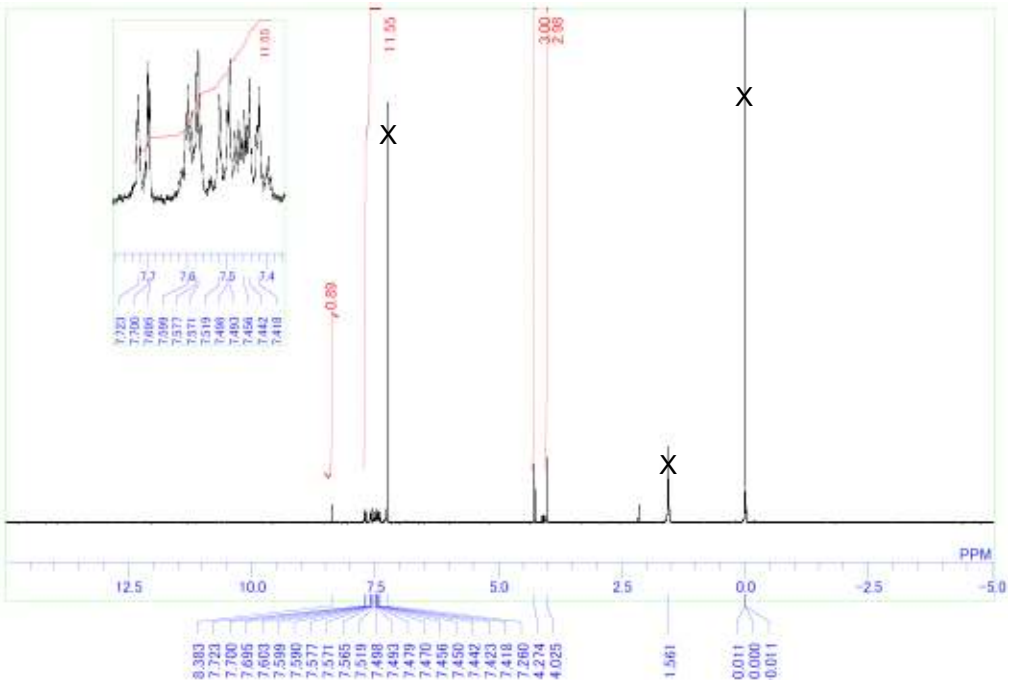


Figure S4. ^{1}H NMR of **M2** in $CDCl_3$.

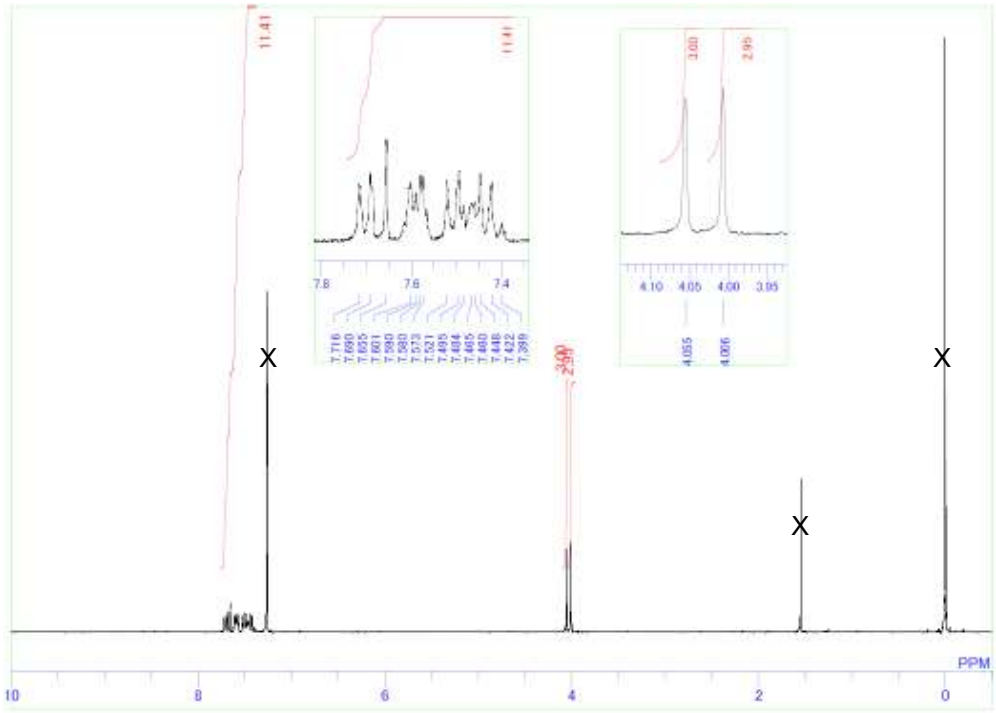


Figure S5. ^{1}H NMR of **M3** in $CDCl_3$.

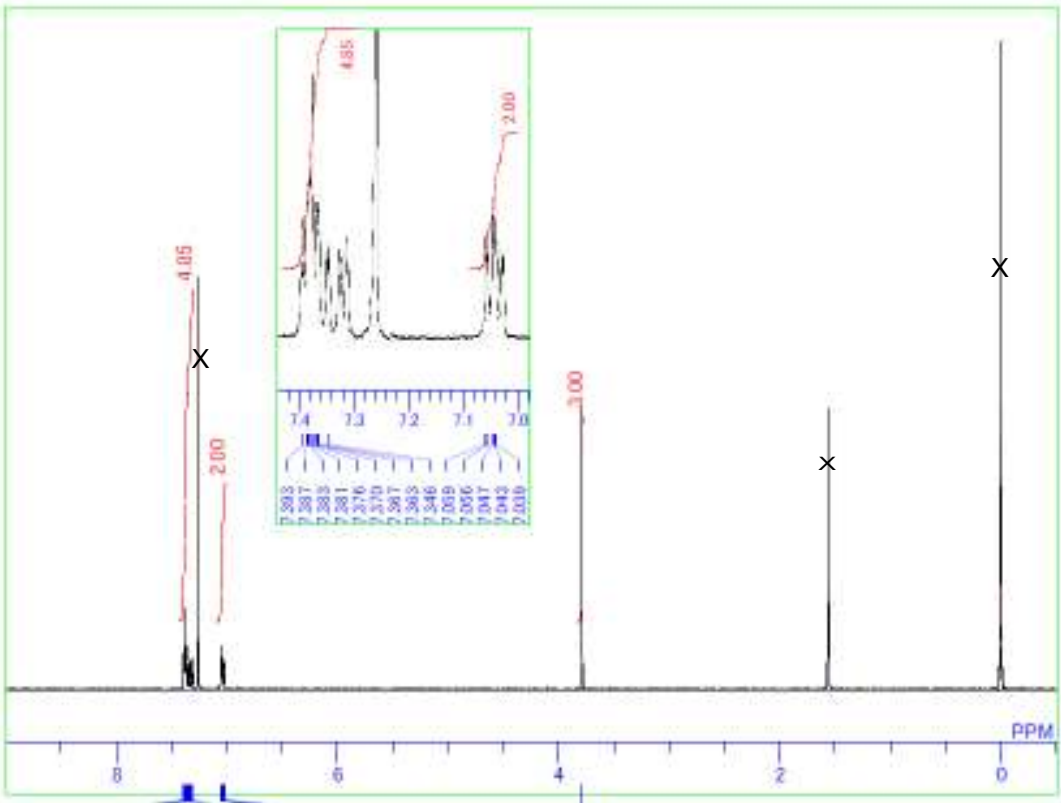


Figure S6. ^{1}H NMR of **M4** in $CDCl_3$.

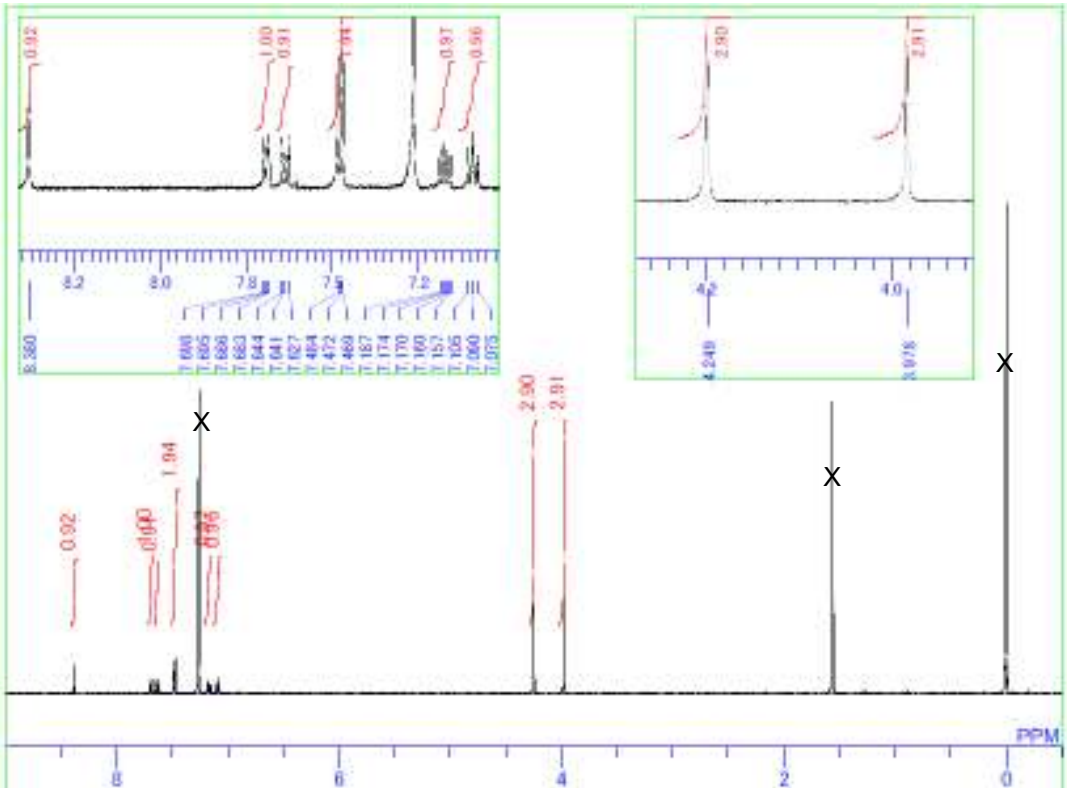


Figure S7. ^{1}H NMR of **M5** in $CDCl_3$.

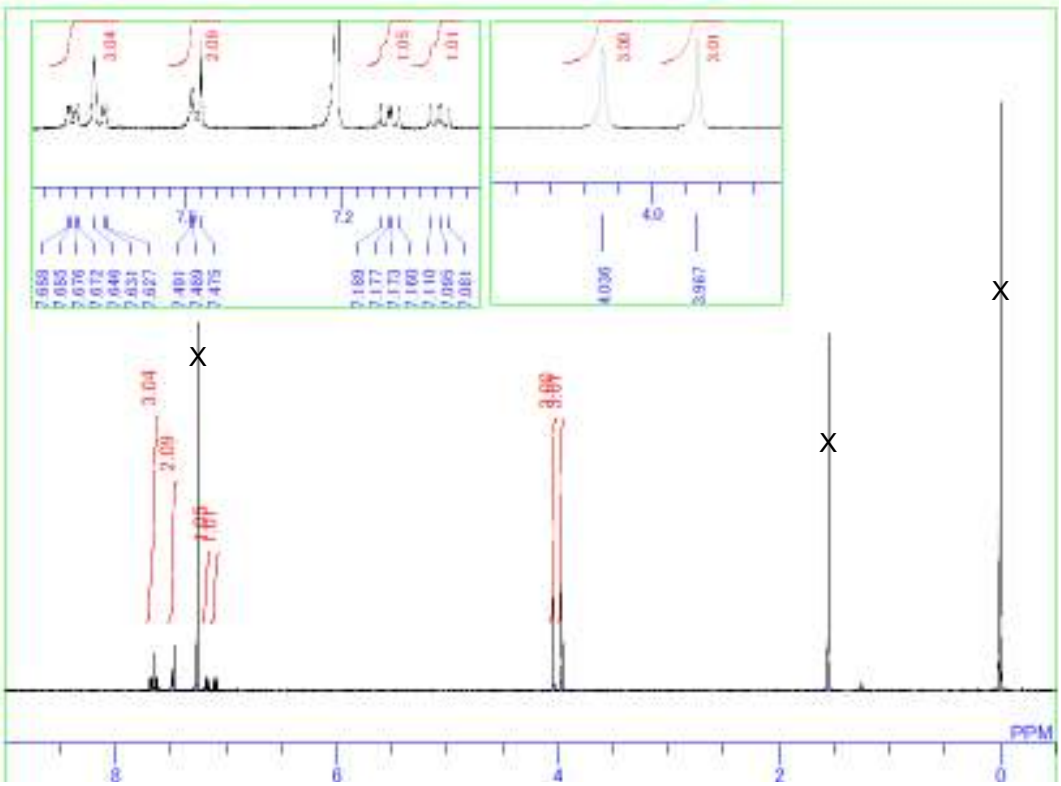
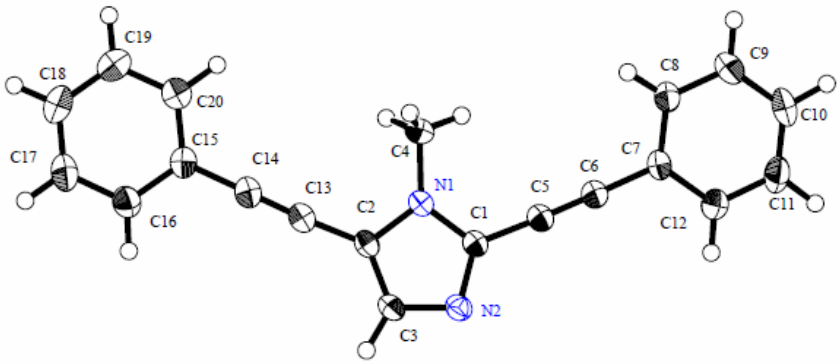
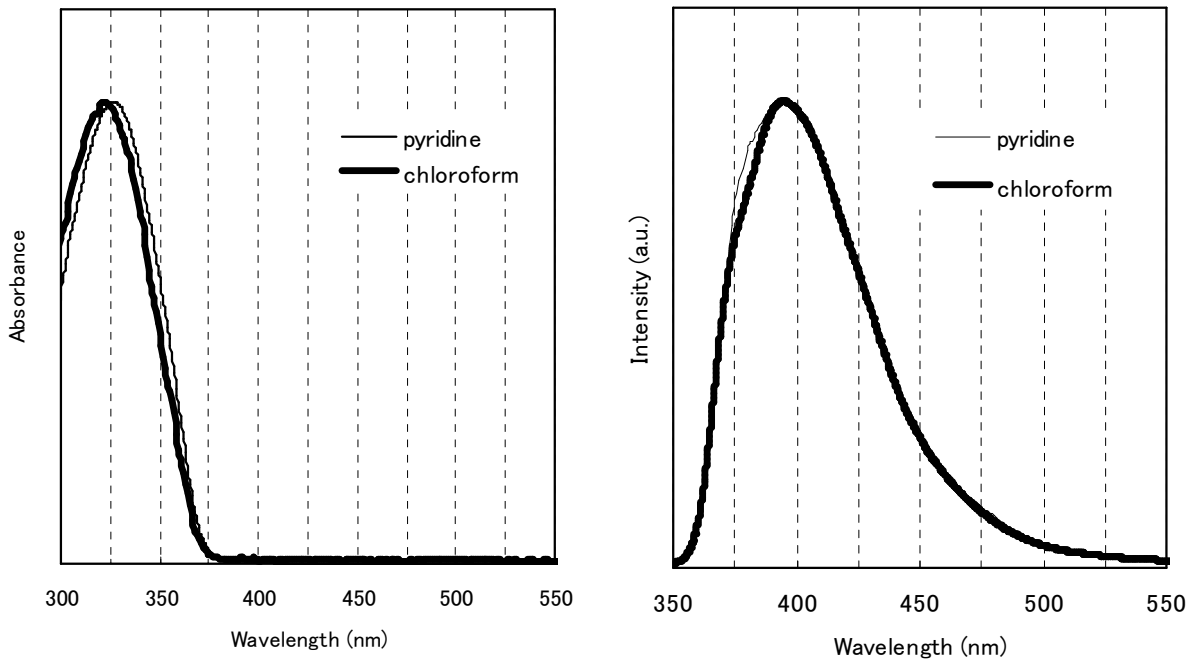


Figure S8. ^{1}H NMR of **M6** in $CDCl_3$.

(2) X-ray Crystal Structure of **M1**



(3) Absorption and fluorescence spectra of **M2** in pyridine and chloroform



(4) DFT Calculations

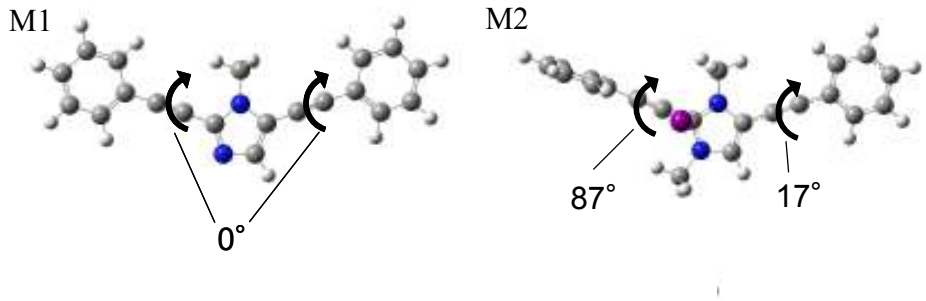


Figure S9. DFT-based optimized structures of **M1**-**M2** and dihedral angles between phenyl rings and imidazole ring or phenyl rings and imidazolium ring.

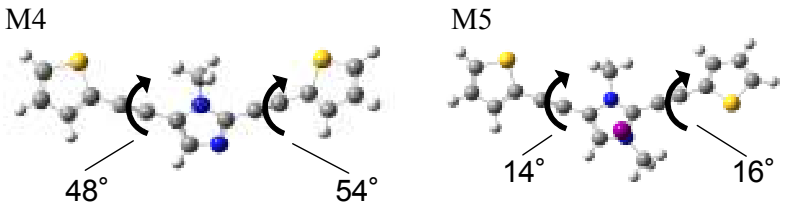


Figure S10. DFT-based optimized structures of **M4**-**M5** and dihedral angles between phenyl rings and imidazole ring or phenyl rings and imidazolium ring.

Table S1. Calculated UV-vis Absorption Wavelength and Oscillator Strength of Model Compounds and Methylated Model Compounds with Counter Anion

Compounds	UV-vis calcd. ($\lambda_{calcd.}$, nm)	Oscillator strength
M1	370	1.5770
M2 (Iodide)	317	1.0843
M4	361	0.9131
M5 (Iodide)	393	1.4184

Full text of reference 15.

(15) *Gaussian 03*, Revision D.01: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A. Jr., Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H. ; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; 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.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Dannenberg, P. Salvador, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A.; Gaussian 03, version 6.1; Gaussian, Inc., Pittsburgh, PA, 2003.