

Molecular Design and Synthesis of Hetero-trichromophore for Enhanced Nonlinear Optical Activity

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Supporting Information:

1. Full author list of reference 37.

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; 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.; 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.; Salvador, P.; Dannenberg, 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*, Revision B.05; Gaussian Inc., Pittsburgh, PA, 2003.

2. The UV-vis absorption spectra of doped polymer films and **1**, **2** and **HT-1** at different concentrations in solutions.

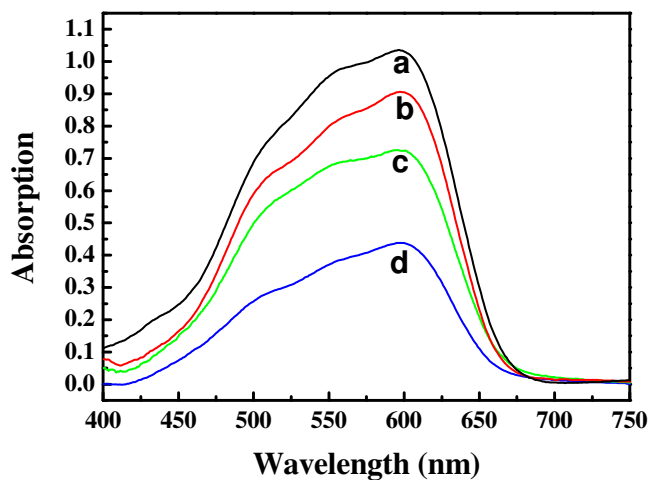


Figure S1. UV-vis spectra of **HT-1** in PVPh: a, 20 wt %; b, 16 wt %; c, 12.8 wt %; d, 9 wt %.

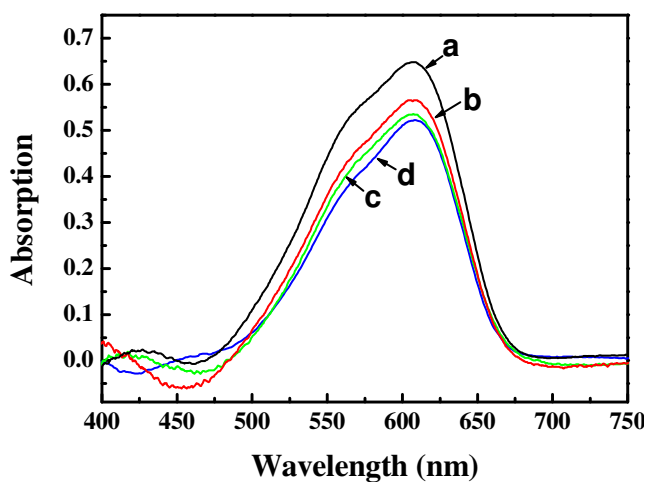


Figure S2. UV-vis spectra of chromophore **1** in PVPh: a, 20 wt %; b, 16 wt %; c, 12.8 wt %; d, 10 wt %.

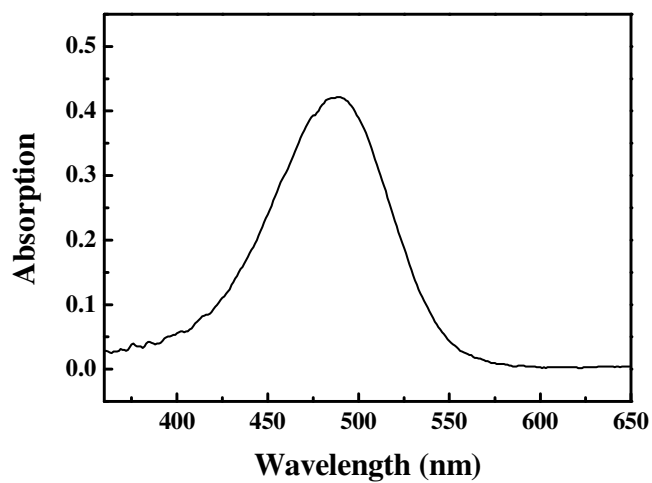


Figure S3. UV-vis spectra of chromophore **2** in PVPh: 7.0 wt %.

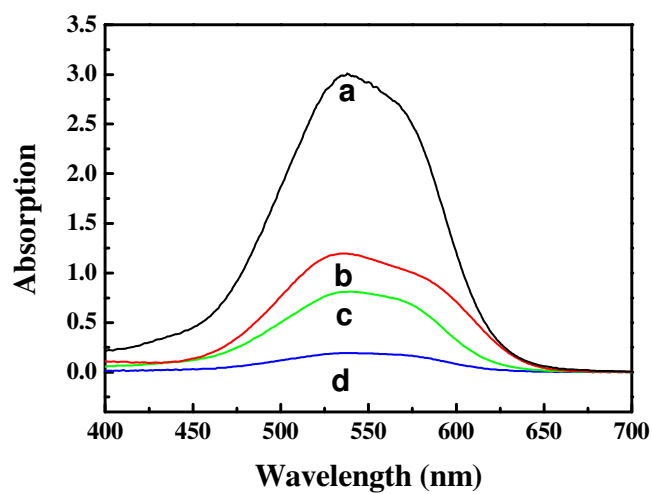


Figure S4. UV-vis spectra of **HT-1** in CHCl₃: a, 2×10^{-5} mol/l; b, 1×10^{-5} mol/l; c, 5×10^{-6} mol/l; d, 1×10^{-6} mol/l.

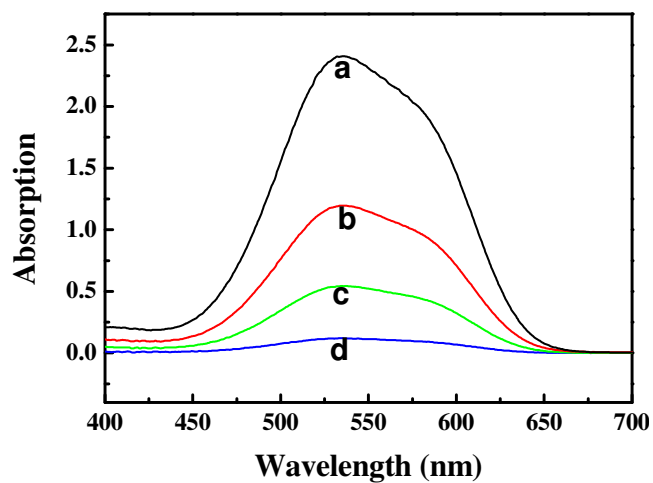


Figure S5. UV-vis spectra of **HT-1** in DMF: a, 2×10^{-5} mol/l; b, 1×10^{-5} mol/l; c, 5×10^{-6} mol/l; d, 1×10^{-6} mol/l.

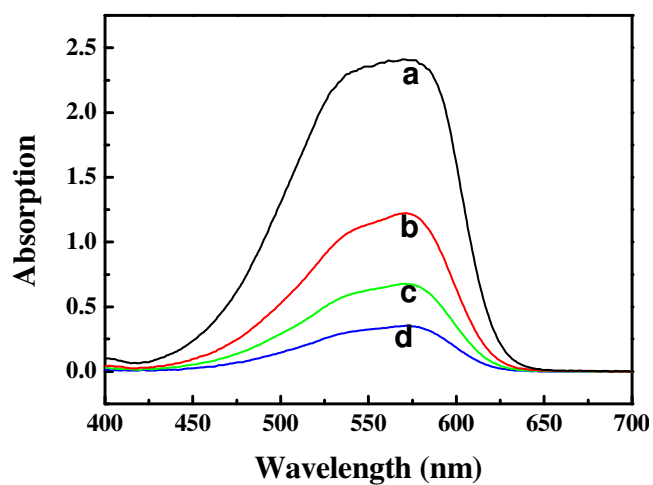


Figure S6. UV-vis spectra of chromophore **1** in CHCl₃: a, 5×10^{-5} mol/l; b, 2×10^{-5} mol/l; c, 1×10^{-5} mol/l; d, 5×10^{-6} mol/l.

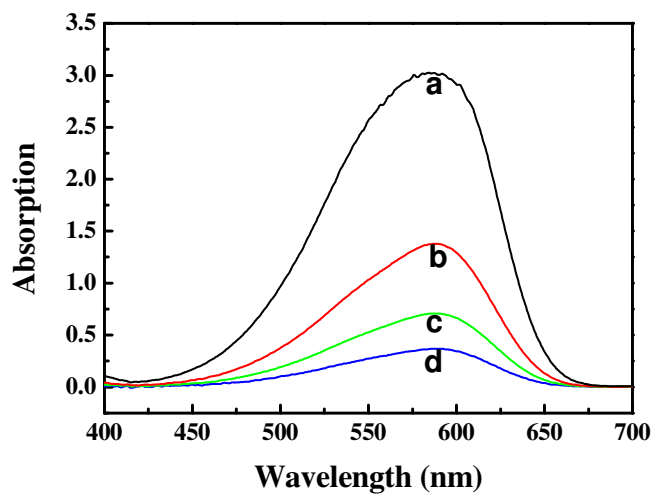


Figure S6. UV-vis spectra of chromophore **1** in DMF: a, 5×10^{-5} mol/l; b, 2×10^{-5} mol/l; c, 1×10^{-5} mol/l; d, 5×10^{-6} mol/l.

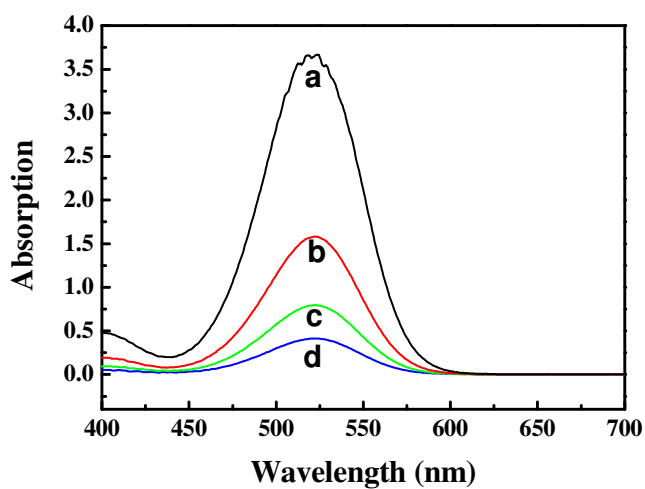


Figure S7. UV-vis spectra of chromophore **2** in DMF: a, 5×10^{-5} mol/l; b, 2×10^{-5} mol/l; c, 1×10^{-5} mol/l; d, 5×10^{-6} mol/l.