Electronic Supplementary Material (ESI) for RSC Advances. This journal is © The Royal Society of Chemistry 2014

Metal-free synthesis of 1,3,5-trisubstituted benzenes by the

cyclotrimerization of enaminones or alkynes in water

Jie-Ping Wan,**, Yunfang Lin Kaikai Hu and Yunyun Liu**,

^aCollege of Chemistry and chemical engineering, Jiangxi Normal University, Nanchang 330022, P.

R. of China.

^bKey laboratory of functional small organic molecules, ministry of education, Jiangxi Normal

University, Nanchang 330022, P. R. of China.

Email: wanjieping@gmail.com; chemliuyunyun@gmail.com

General experimental information

All experiments were carried out at open atmosphere, enaminones used in the

experiment were prepared following literature method, and all other chemicals were

obtained from commercial resource and used without further purification. Deionized

water was used for reactions involving water as solvent. ¹H and ¹³C NMR were

recorded in 400 HMz apparatus (AVANCE 400, Bruker) or 600 MHz apparatus

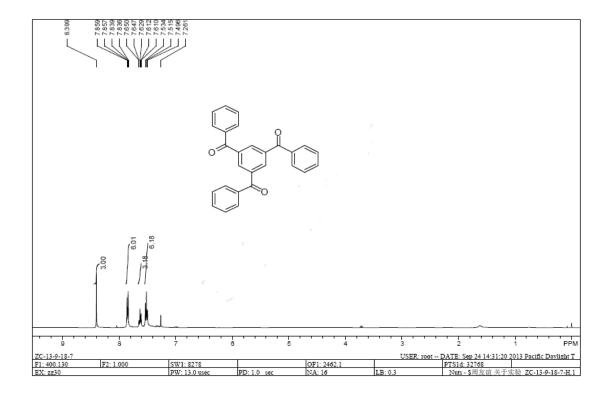
(600MHz DD2, Agilent). The chemical shifts were reported in ppm using TMS as

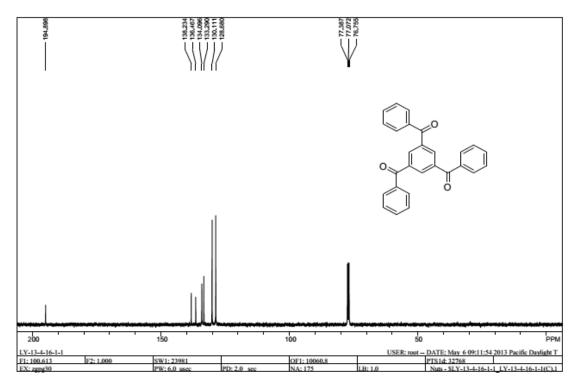
internal standard. Melting points were tested in X-4A instrument without correcting

temperature, IR were measured in KBr method and the HRMS were obtained under

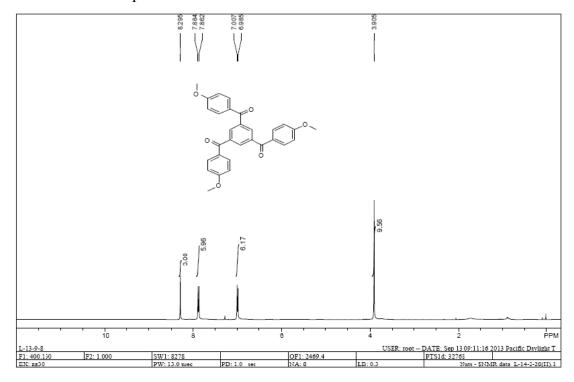
ESI model.

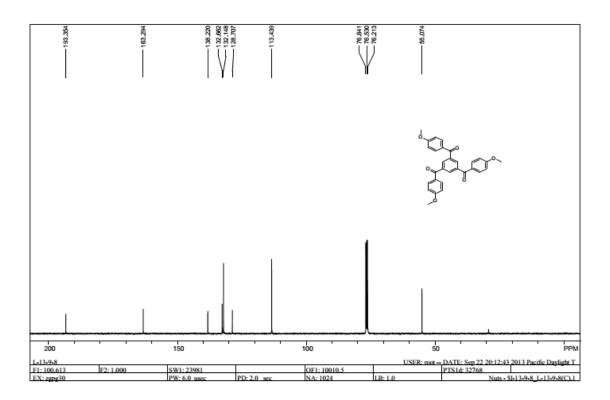
¹H and ¹³C NMR spectra of **3a**



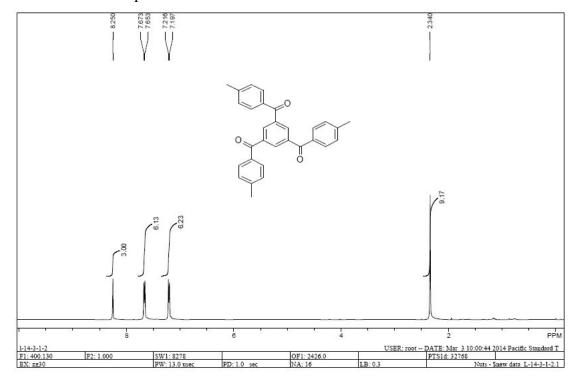


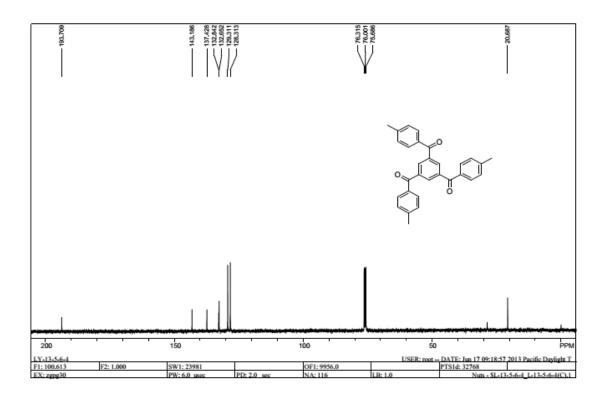
¹H and ¹³C NMR spectra of **3b**



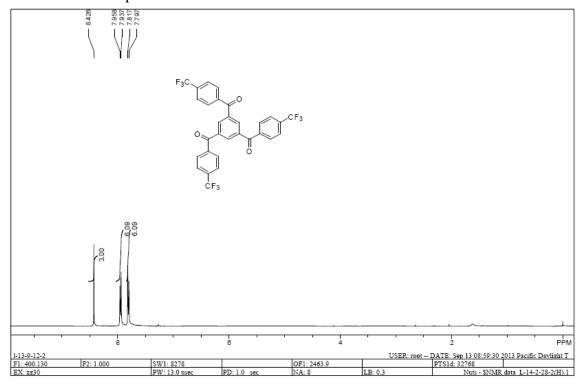


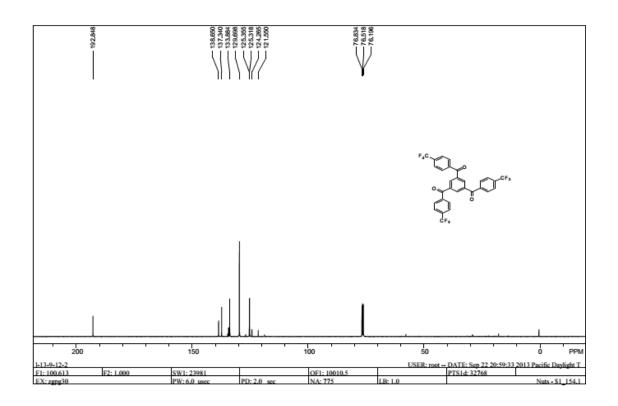
 ^{1}H and ^{13}C NMR spectra of 3c



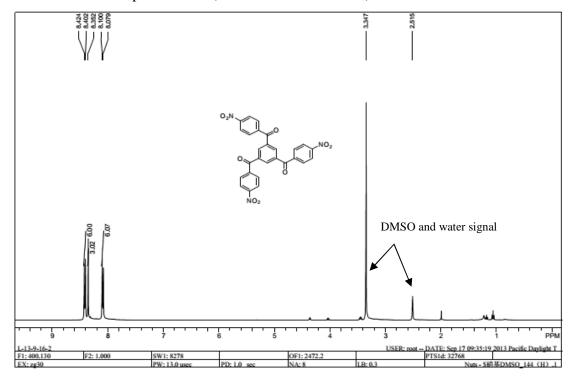


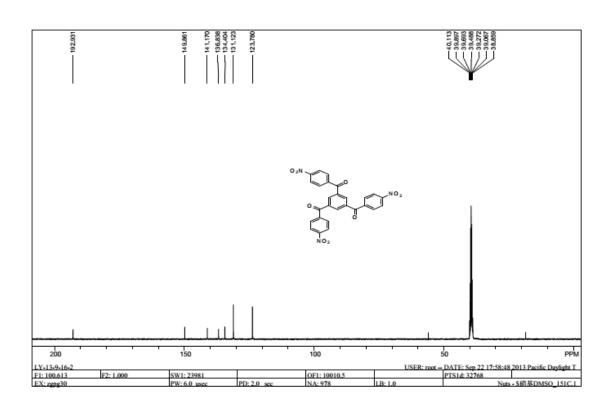
¹H and ¹³C NMR spectra of **3d**



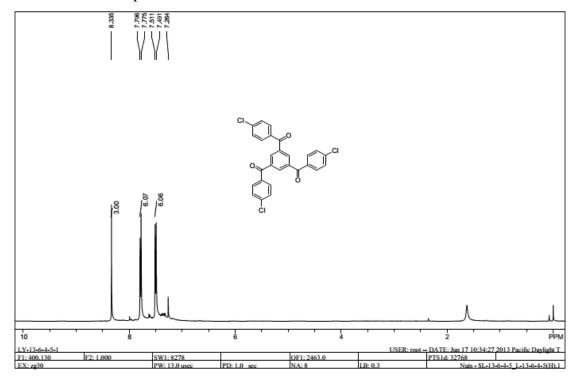


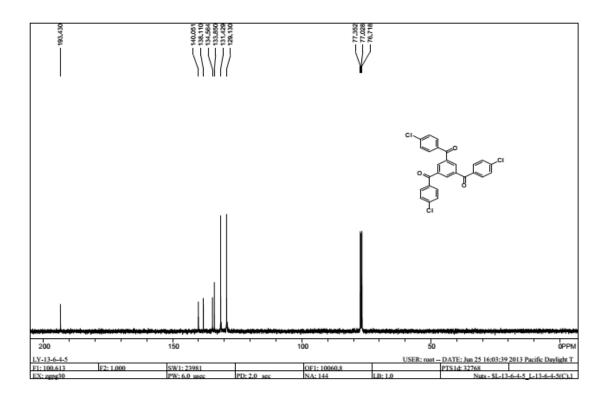
 1 H and 13 C NMR spectra of **3e** (Measured in DMSO- d_{6})



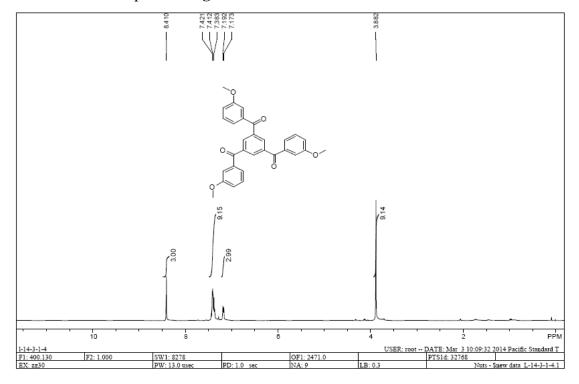


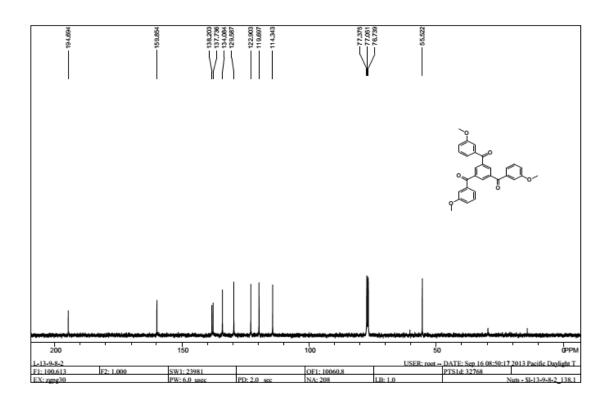
¹H and ¹³C NMR spectra of **3f**



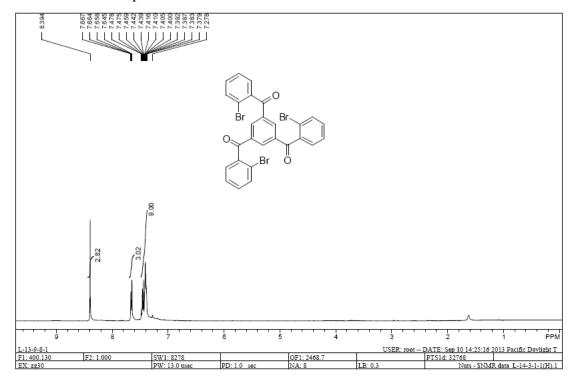


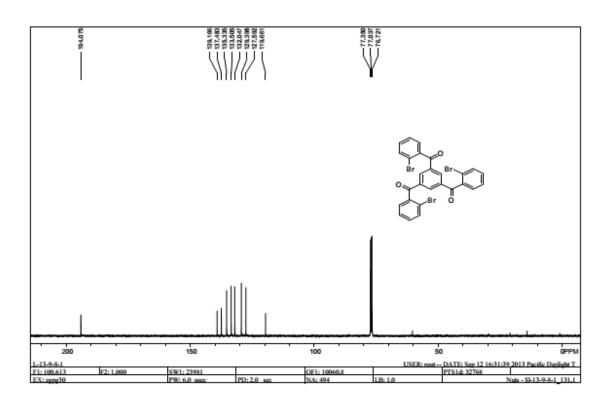
¹H and ¹³C NMR spectra of **3g**



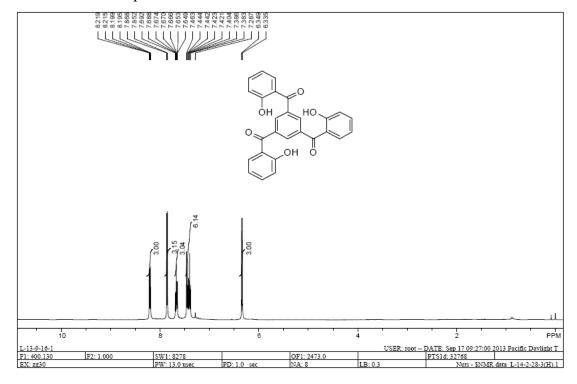


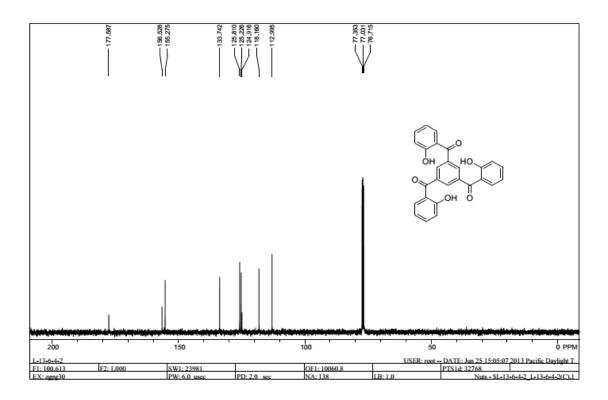
¹H and ¹³C NMR spectra of **3h**



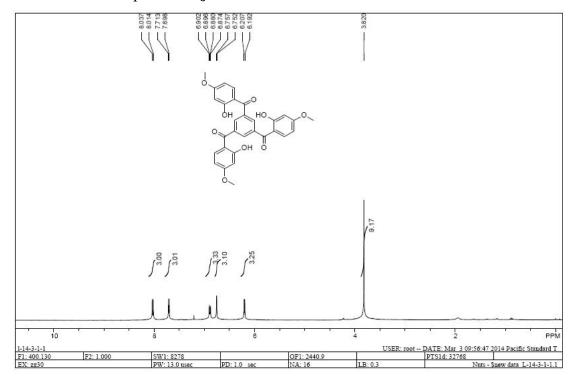


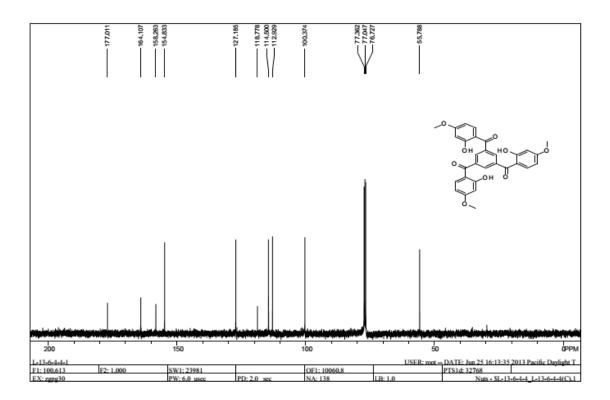
¹H and ¹³C NMR spectra of **3i**



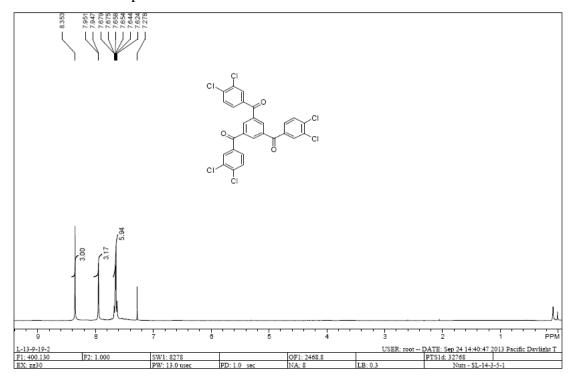


¹H and ¹³C NMR spectra of **3j**

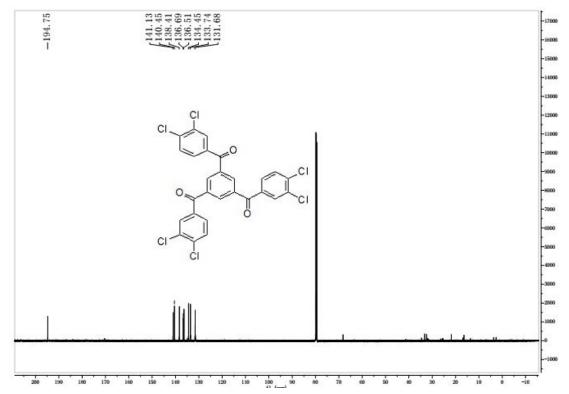




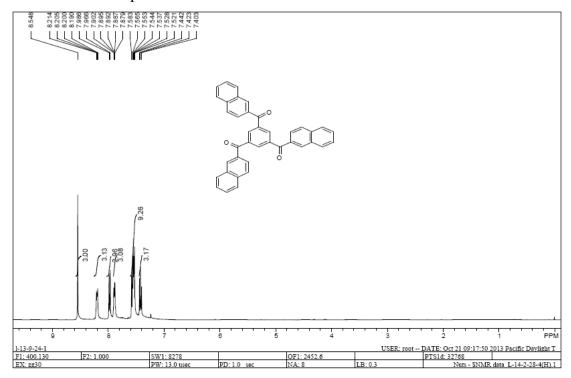
¹H and ¹³C NMR spectra of **3k**



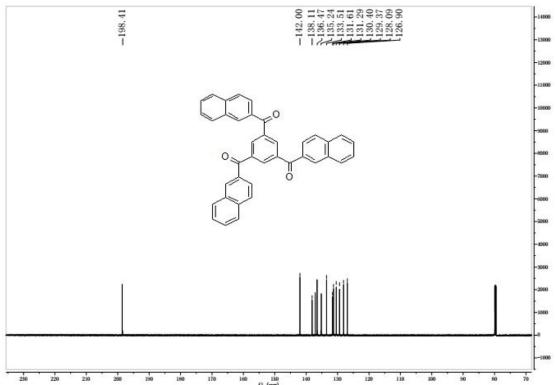
$^{13}\mbox{C}$ NMR was recorded in 600 MHz apparatus



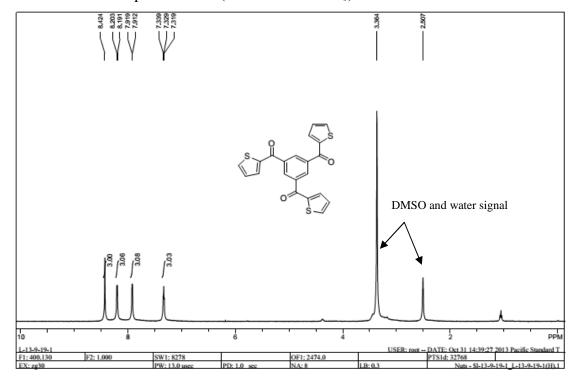
¹H and ¹³C NMR spectra of **31**

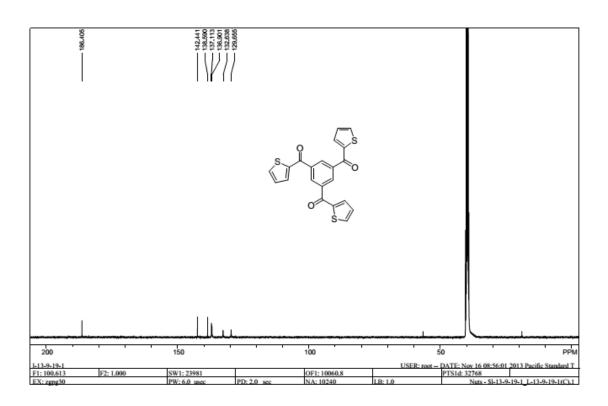


$^{13}\mbox{C}$ NMR was recorded in 600 MHz apparatus

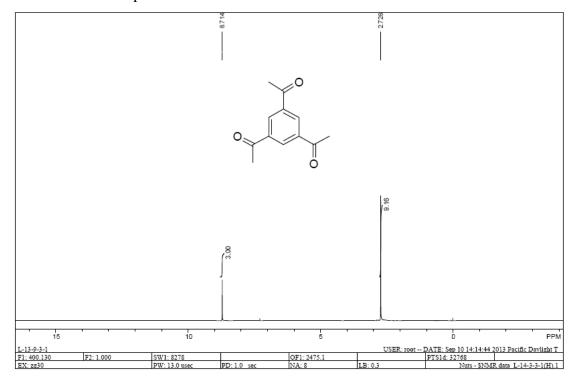


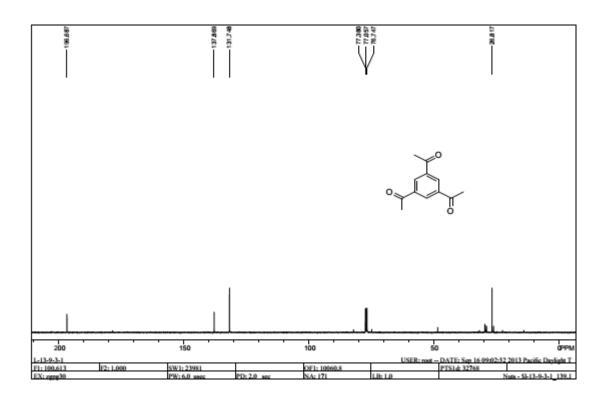
 1 H and 13 C NMR spectra of **3m** (tested in DMSO- d_6)



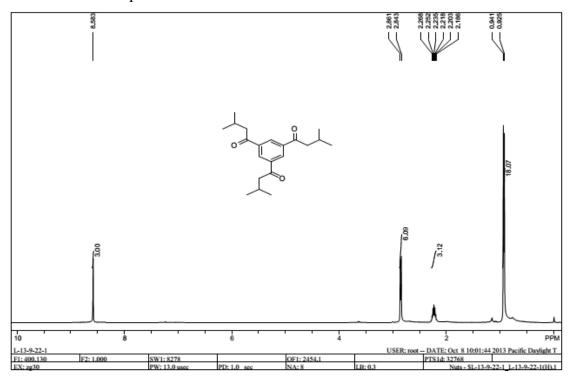


¹H and ¹³C NMR spectra of **3n**

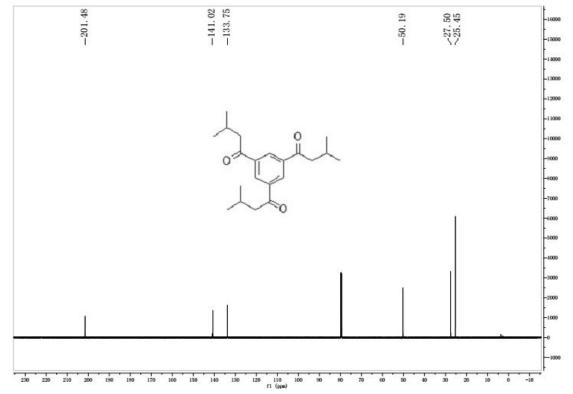




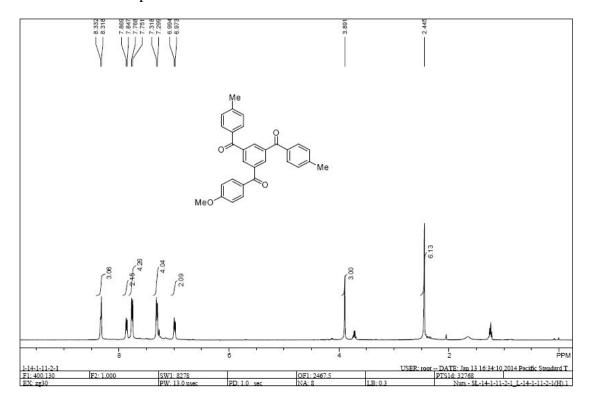
¹H and ¹³C NMR spectra of **30**

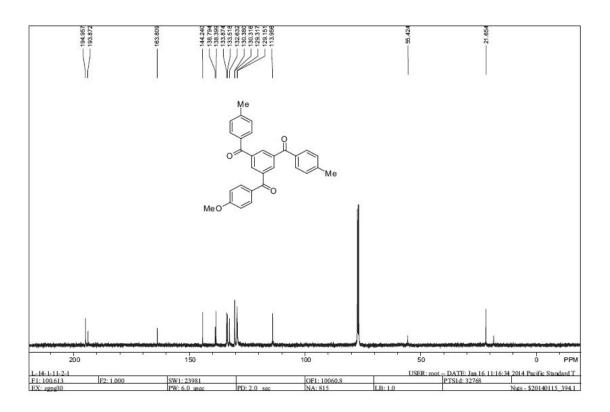


¹³C NMR was recorded in 600 MHz apparatus

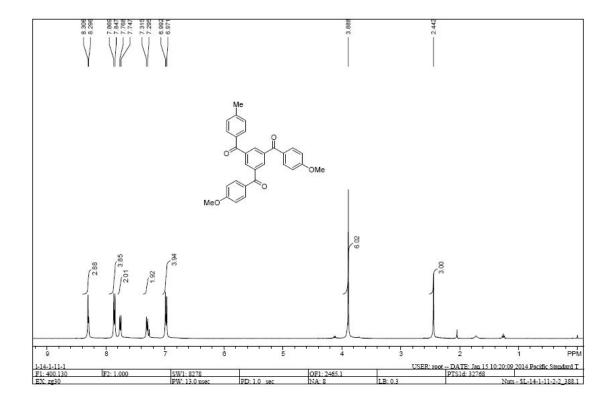


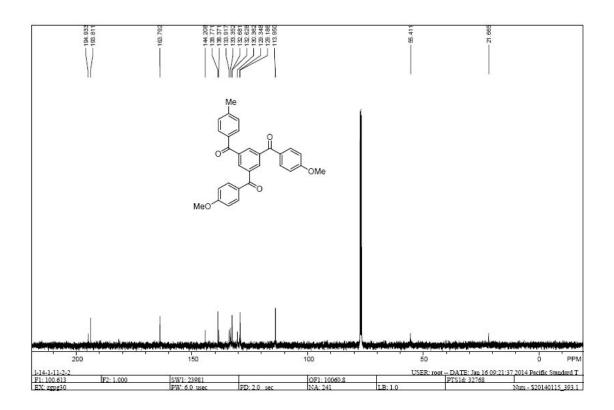
¹H and ¹³C NMR spectra of **3cb**

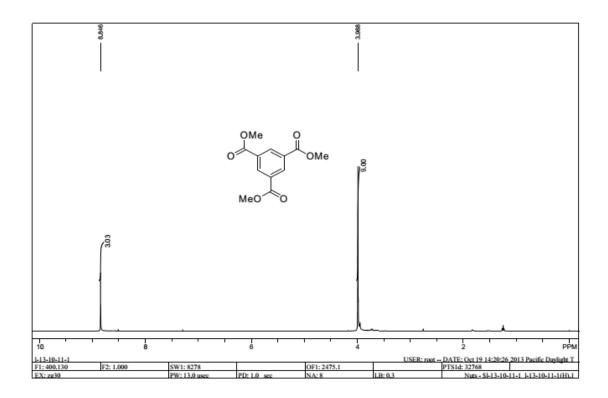




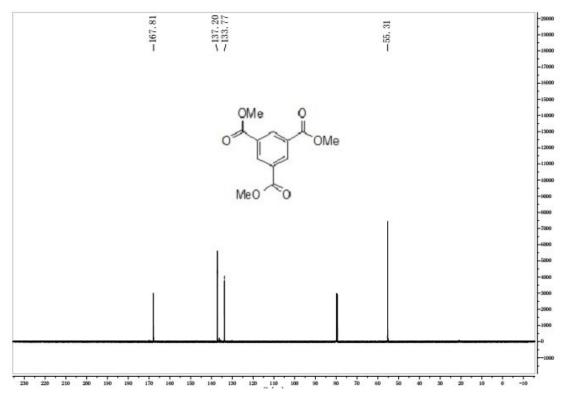
¹H and ¹³C NMR spectra of **3bc**



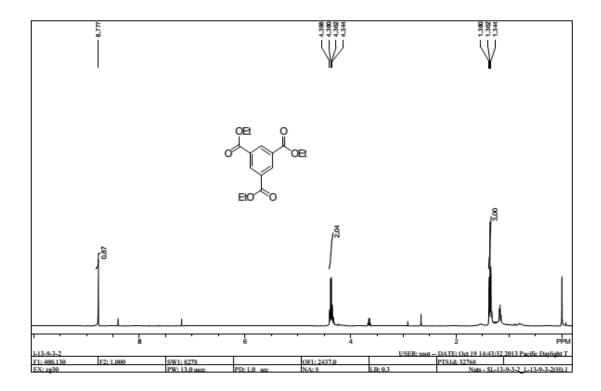




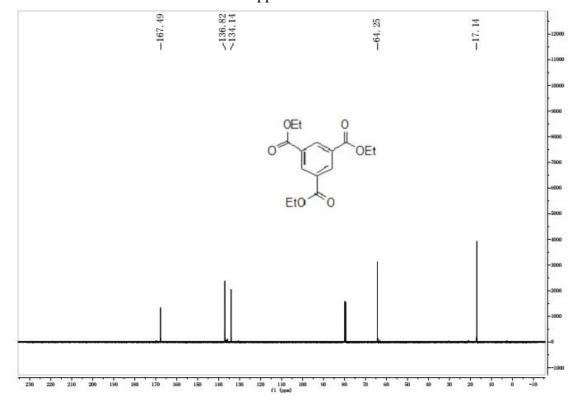
$^{13}\mbox{C}$ NMR was recorded in 600 MHz apparatus



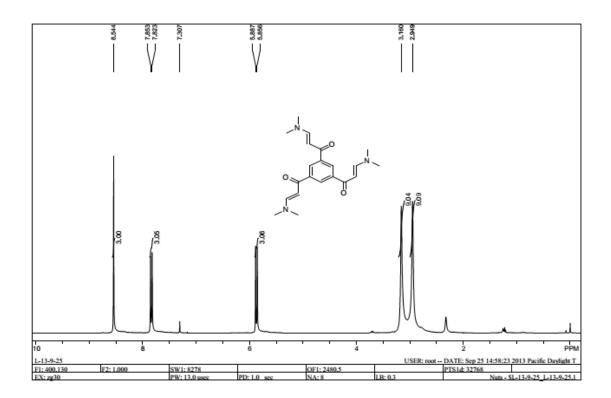
¹H and ¹³C NMR spectra of **7b**



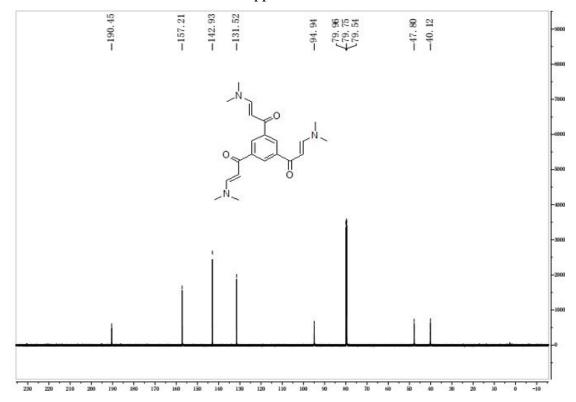
$^{13}\mathrm{C}$ NMR was recorded in 600 MHz apparatus



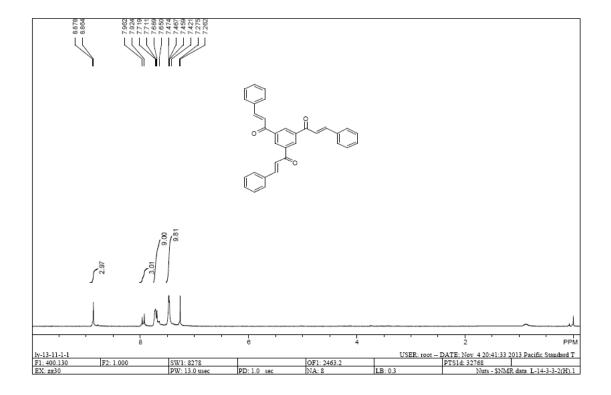
¹H and ¹³C NMR spectra of **9**

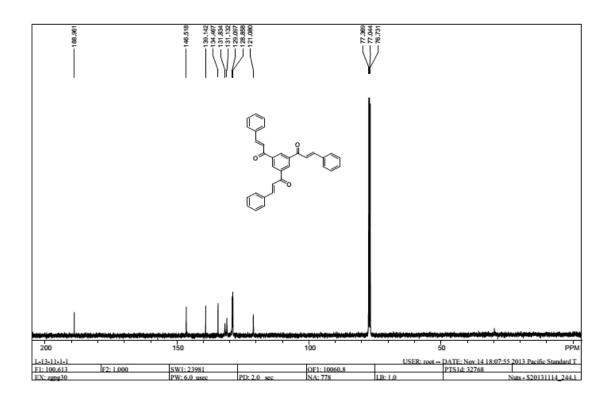


¹³C NMR was recorded in 600 MHz apparatus

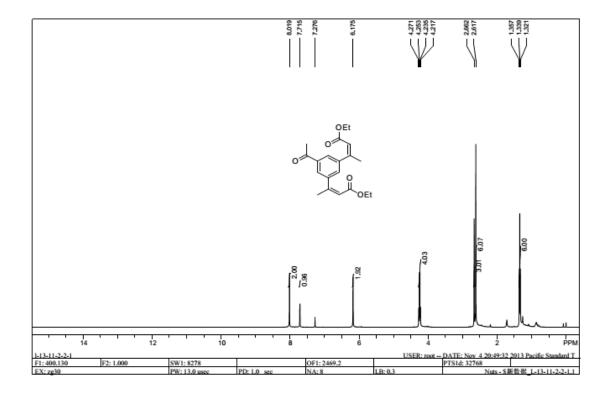


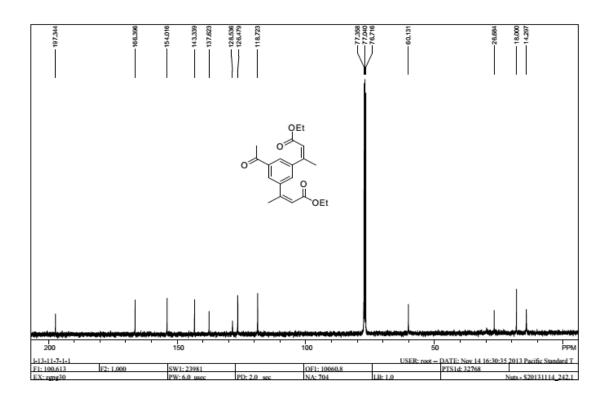
¹H and ¹³C NMR spectra of **10**





¹H and ¹³C NMR spectra of **12a**





¹H and ¹³C NMR spectra of **12b**

