

**Supporting Information For:**

**$\beta$ -Iminoenolate Boron Complex with Terminal Triphenylamine**

**Exhibiting Polymorphism and Mechanofluorochromism**

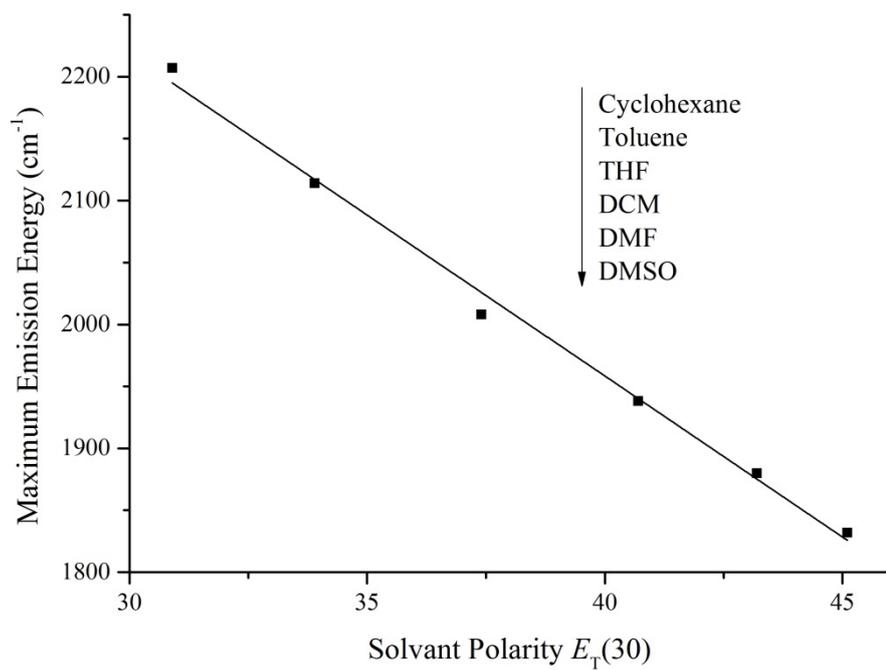
Table 1. Photophysical data of **TP**.

solvent	$E_T(30)$ (kcal/mol)	$\lambda_{\text{abs}}$ (nm) ( $\epsilon$ ) <sup>a</sup>	$\lambda_{\text{em}}$ (nm)	Stokes shift ( $\text{cm}^{-1}$ )	$\Phi_F$ <sup>b</sup>
cyclohexane	30.9	305 (19219)	453,479	1791	0.77
		419 (42111)			
		437 (38483)			
toluene	33.9	420 (38600)	473	2668	0.78
THF	37.4	299 (18824)	498	4016	0.70
		415 (38384)			
DCM	40.7	300 (18179)	516	4316	0.61
		422 (38197)			
DMF	43.2	299 (18860)	532	5241	0.44
		416 (37489)			
DMSO	45.1	299 (14200)	547	5700	0.38
		417 (35277)			

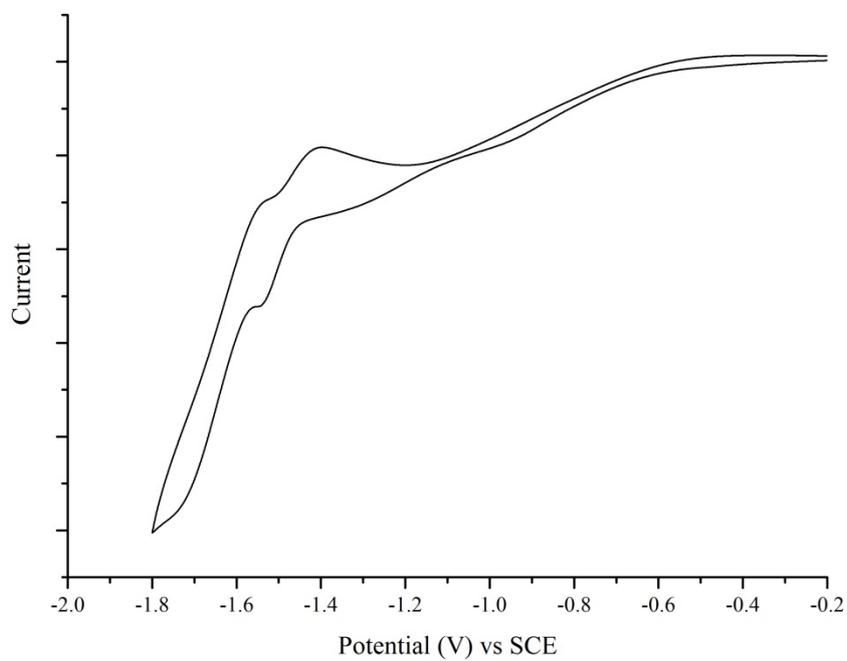
<sup>a</sup>  $\text{M}^{-1}\text{cm}^{-1}$ ; <sup>b</sup> The fluorescence quantum yield ( $\Phi_F$ ) of **TP** was measured using 9,10-diphenylanthracene in benzene ( $\Phi_F = 0.85$ ) as standard.



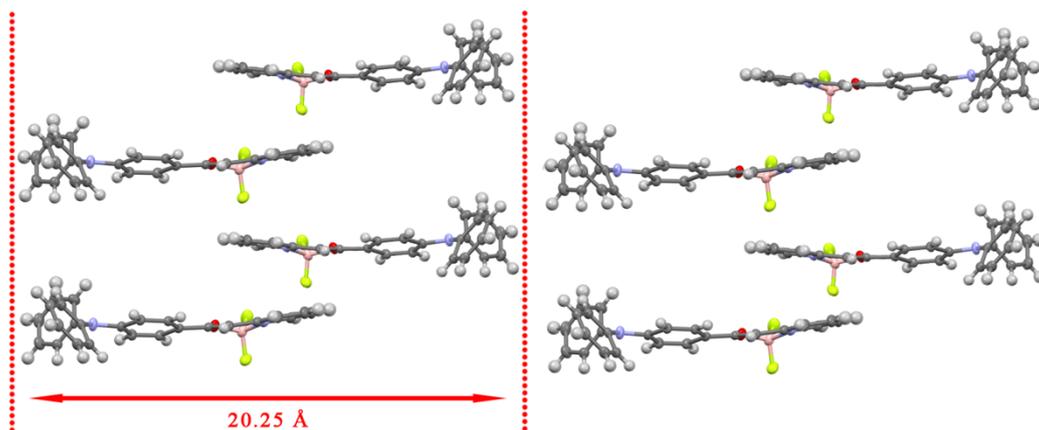
**Figure S1** Photos of **TP** in cyclohexane, toluene, THF, DCM, DMF and DMSO (from left to right) under UV light.



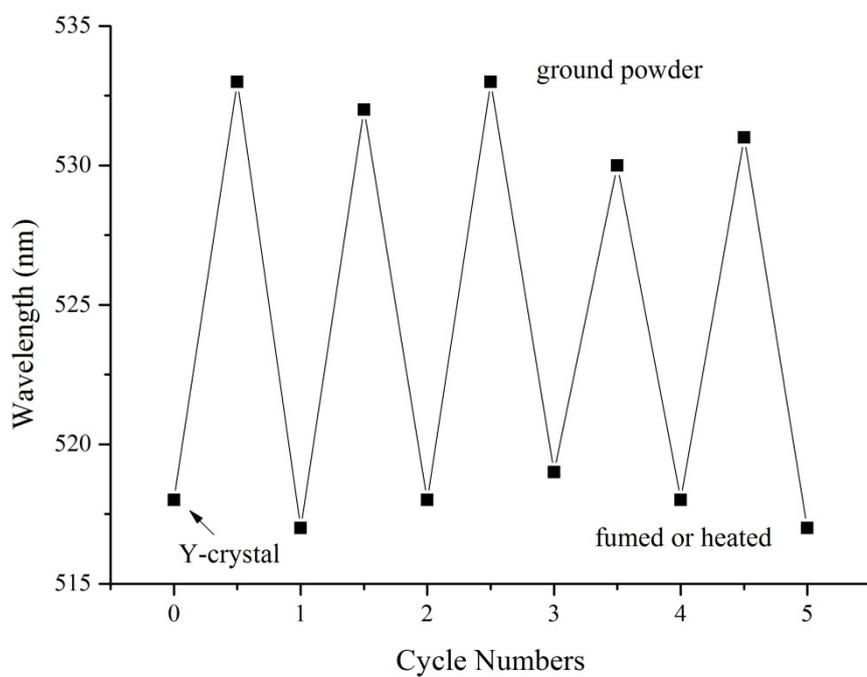
**Figure S2** The plot for the maximum fluorescence emission energy of **TP** vs the solvent polarity.



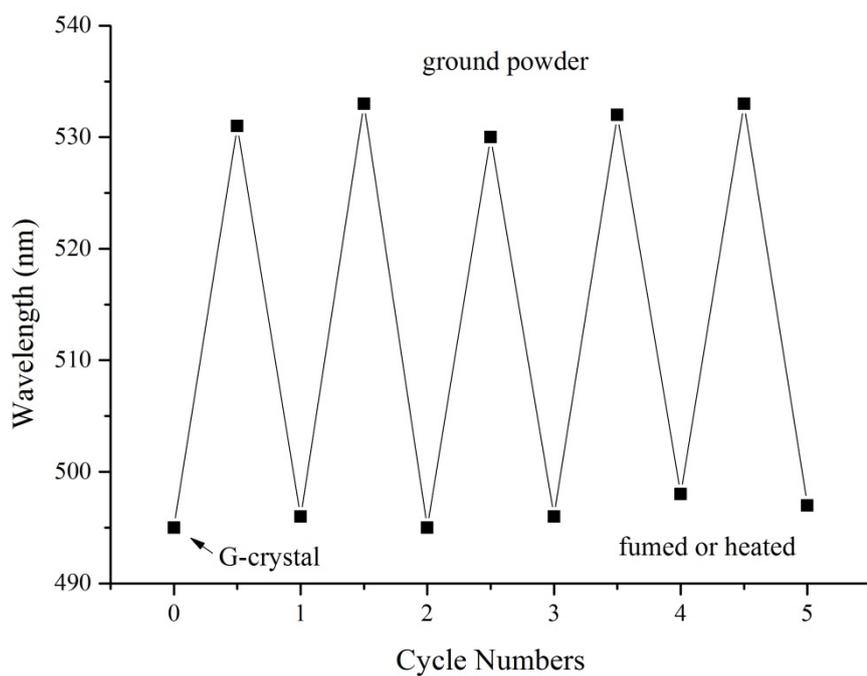
**Figure S3** Cyclic voltammograms of **TP** measured in  $\text{CH}_2\text{Cl}_2$  with  $\text{Bu}_4\text{NBF}_4$  (0.1 M) as electrolyte at a scan rate of 50 mV/s.



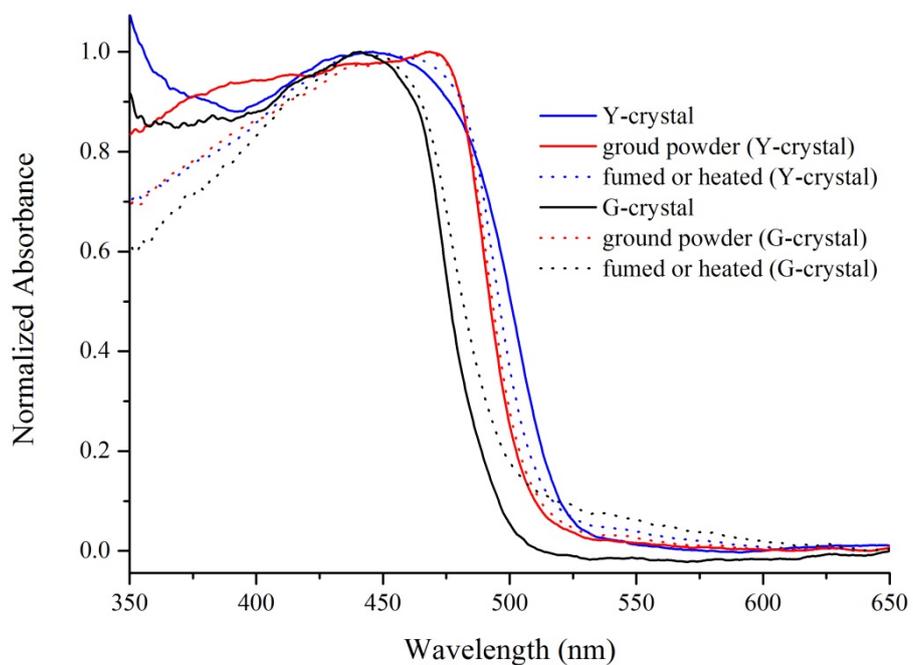
**Figure S4** Proposed molecular packing of TP in G-crystal.



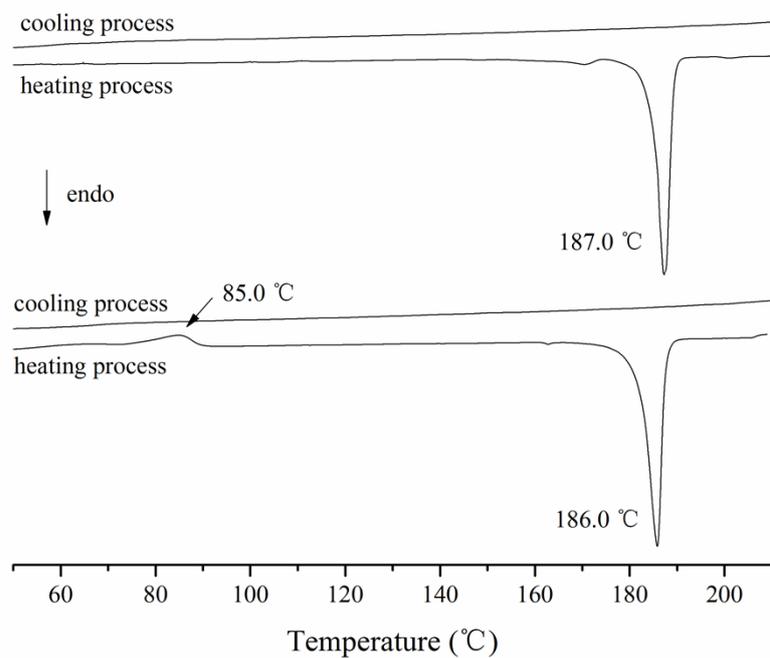
**Figure S5** Maximum fluorescent emission of Y-crystal of TP upon repeating treated by grinding and fuming with  $\text{CH}_2\text{Cl}_2$ .



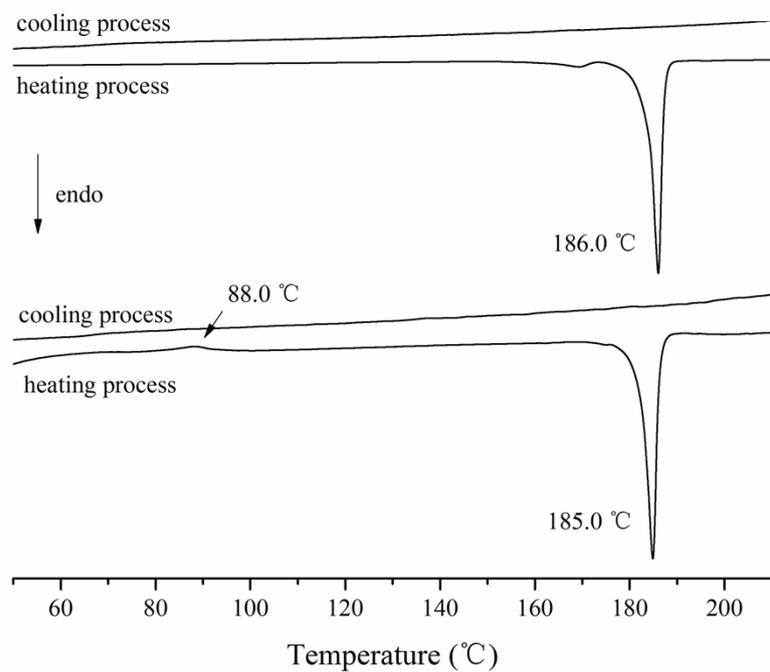
**Figure S6** Maximum fluorescent emission of G-crystal of **TP** upon repeating treated by grinding and fuming with  $\text{CH}_2\text{Cl}_2$ .



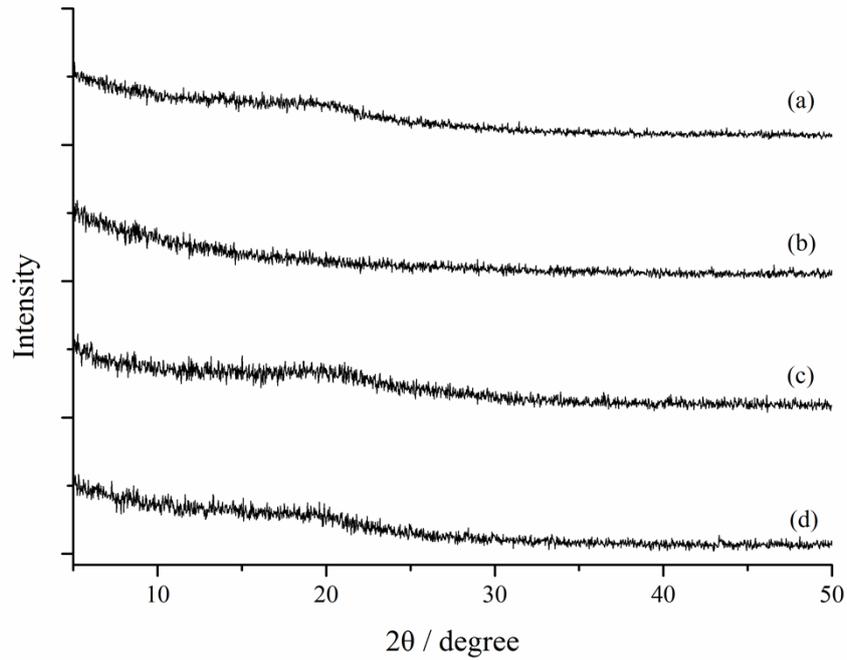
**Figure S7** UV-vis spectra of **TP** in different solid states measured a reflection way.



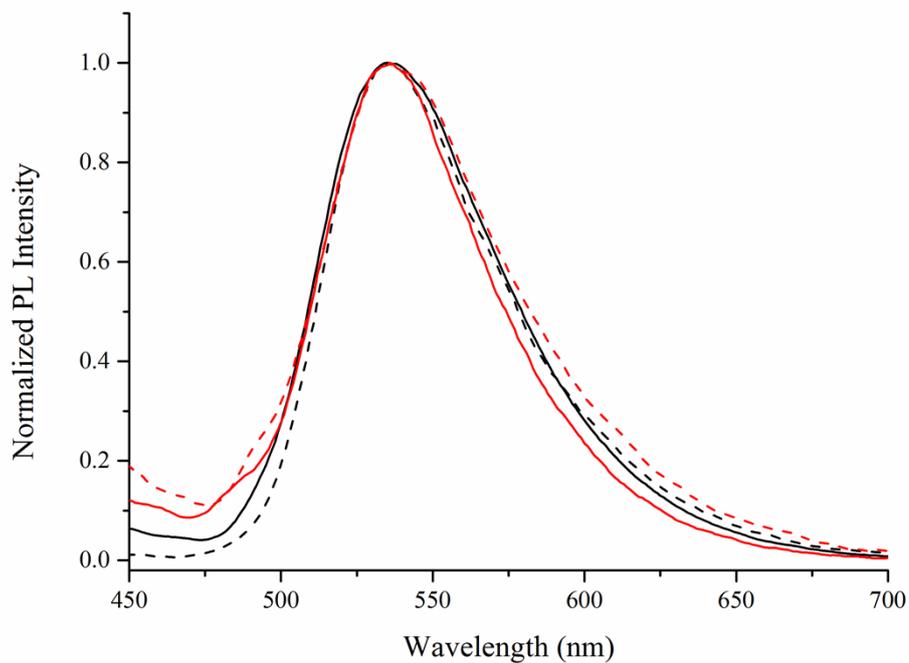
**Figure S8** DSC curves of Y-crystal (above) and ground powder obtained from Y-crystal (below).



**Figure S9** DSC curves of G-crystal (above) and ground powder obtained from G-crystal (below).



**Figure 10** XRD patterns of the high-temperature annealed samples obtained from Y-crystal (a), ground powder of Y-crystal (b), G-crystal (c) and ground powder of G-crystal (d).



**Figure S11** Normalized fluorescence emission spectra of the high-temperature annealed samples obtained from Y-crystal (black line), ground powder of Y-crystal (black dash), G-crystal (red line) and ground powder of G-crystal (red dash).

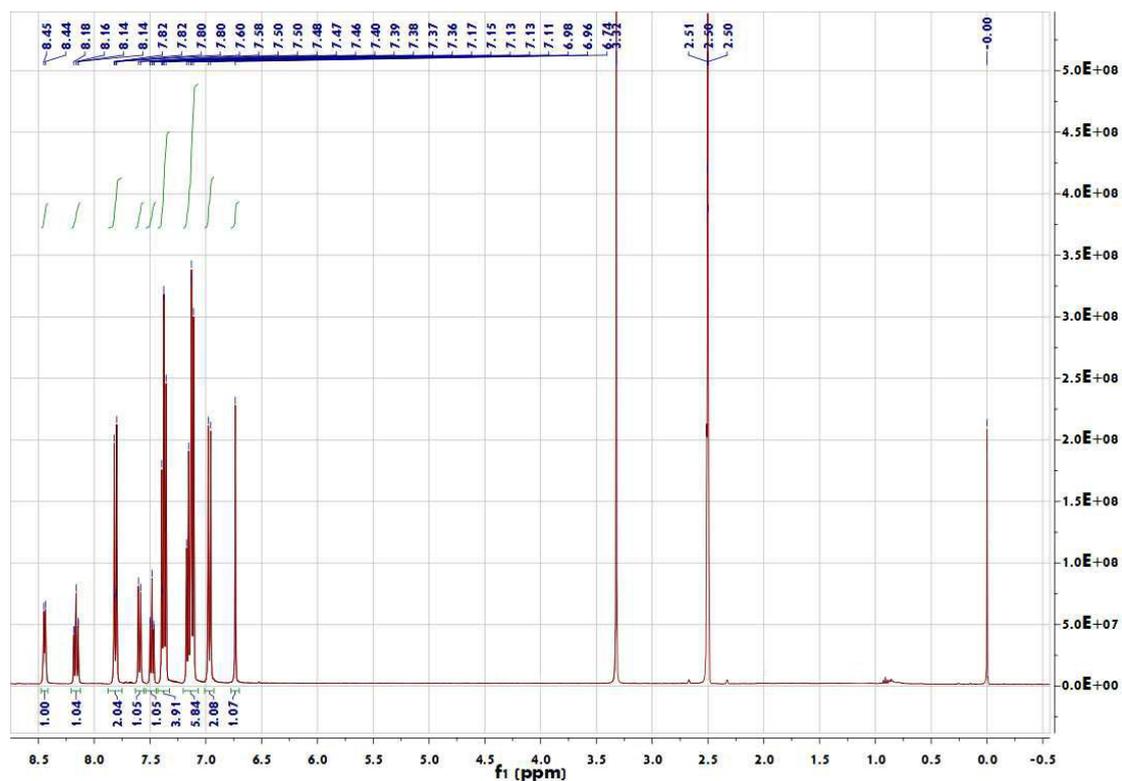


Figure S12  $^1\text{H}$  NMR (400 MHz) spectrum of compound TP in  $\text{DMSO-}d_6$ .

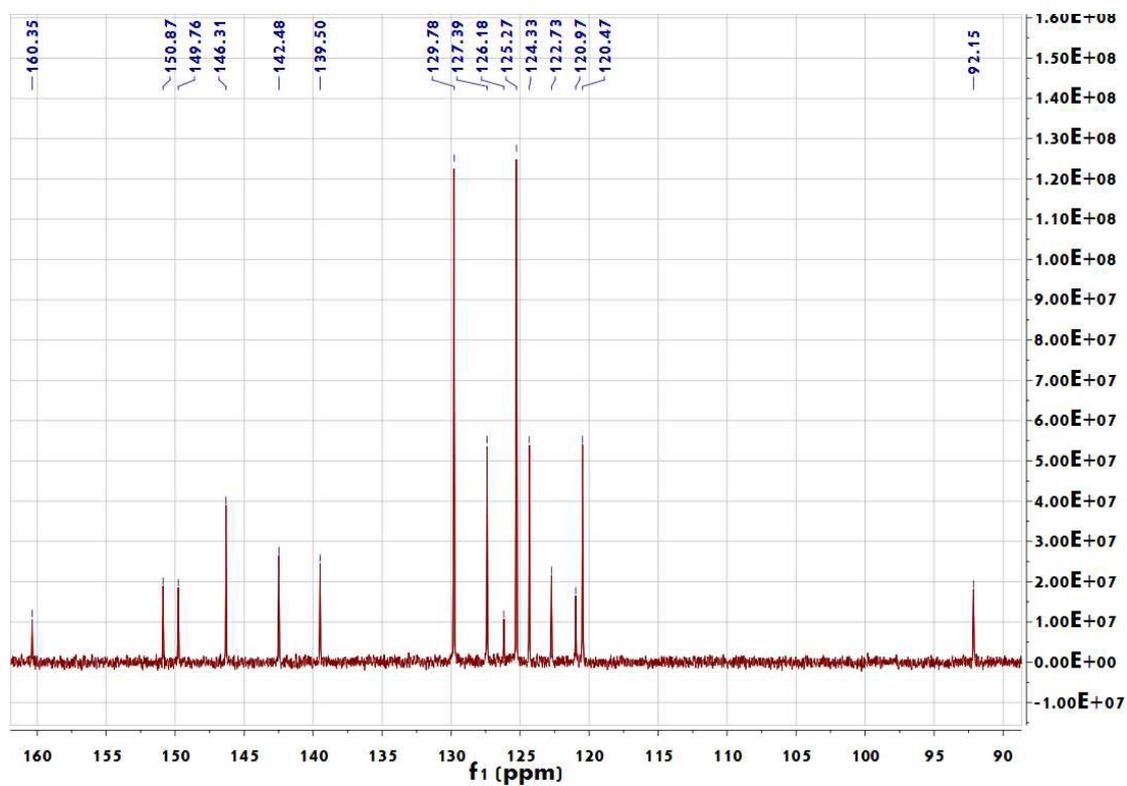
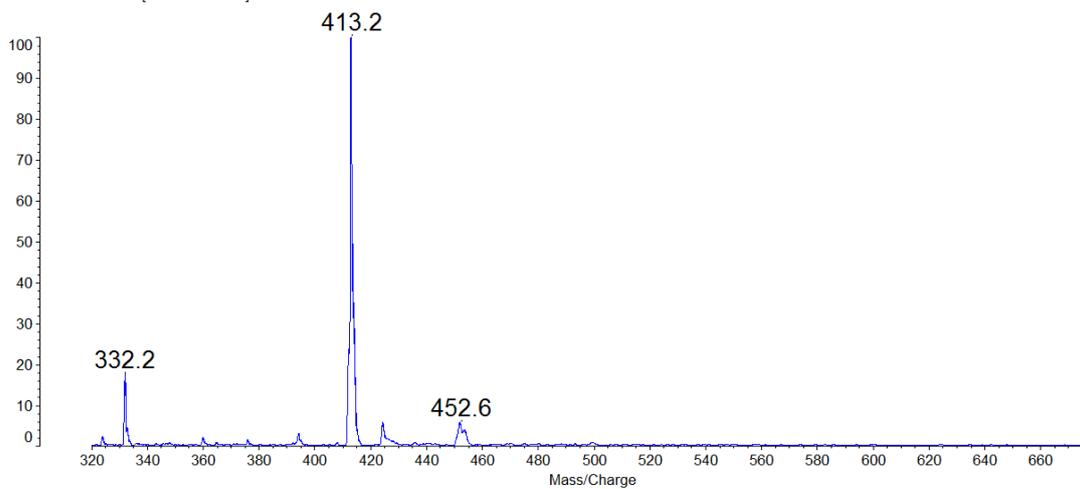


Figure S13  $^{13}\text{C}$  NMR (100 MHz) spectrum of compound TP in  $\text{DMSO-}d_6$ .

Reflectron Mode

Data: LR-66-L0001.M15 29 Mar 2013 16:05 Cal: 30 Mar 2013 9:47  
Kratos PC Axima CFR V2.3.1: Mode default\_linear, Power: 70, P.Ext. @ 412 (bin 57)  
%Int. 338 mV[sum= 4729 mV] Profiles 1-14 Smooth Av 20 -Baseline 80



**Figure S14** MALDI/TOF MS spectrum of compound **TP**.