

*Supporting Informations*

For

**Variation in solvato-, AIE- and mechano-fluorochromic behavior for furanyl  
and thiophenyl-substituted anthranil  $\pi$ -conjugates: role of tiny flanking  
donor groups**

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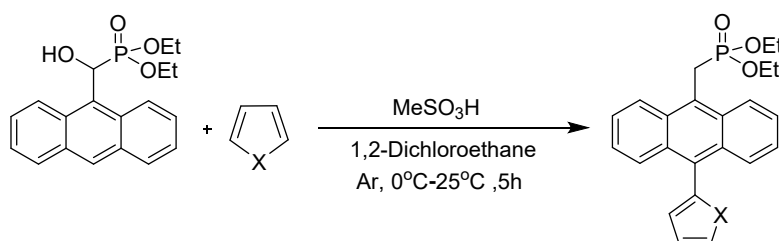
### *Synthesis and Characterization of diethyl ((10-(thiophen-2-yl)anthracen-9-yl)methyl)phosphonate:*

This compound was earlier reported by us.<sup>1</sup>

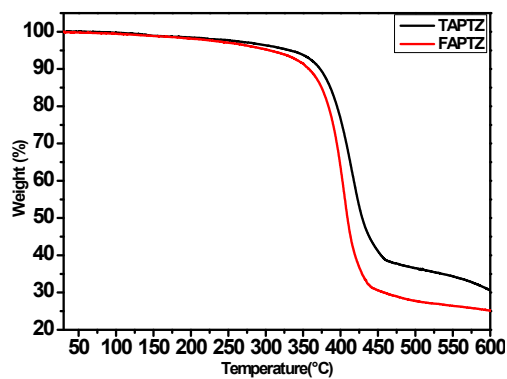
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.41 (d, *J* = 8.9 Hz, 2H), 7.89 (d, *J* = 8.8 Hz, 2H), 7.63 – 7.54 (m, 3H), 7.42 (dd, *J* = 8.7, 6.5 Hz, 2H), 7.31 (dd, *J* = 5.2, 3.4 Hz, 1H), 7.19 (m, 1H), 4.29 (d, *J* = 22.5 Hz, 2H), 4.08 – 3.83 (m, 4H), 1.17 (t, *J* = 7.1 Hz, 6H).

### *Synthesis and Characterization of diethyl ((10-(furan-2-yl)anthracen-9-yl)methyl)phosphonate:*

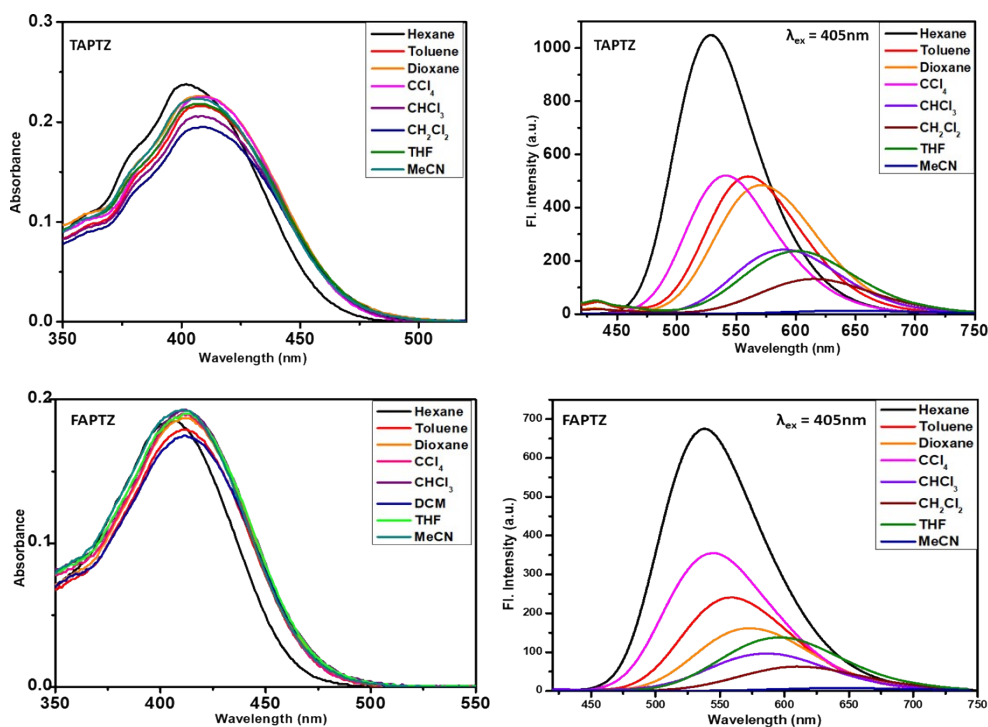
In a 50mL round-bottomed flask, diethyl (anthracen-9-yl(hydroxy)methyl)phosphonate (1.0 g, 2.904mmol) was dissolved in 40ml of dry dichloroethane in ice temperature followed by the addition of methanesulfonic acid (0.565ml, 8.712mmol) and furan (0.211 ml, 2.904 mmol). The reaction was allowed to stir for 5 h. The completion of the reaction was monitored by TLC plate. The reaction mixture was quenched by water and extracted with dichloromethane (20 mL x 3). The organic layer was filtered and dried over anhydrous sodium sulfate and evaporated under reduced pressure. The compound was purified by column chromatography (100-200 mesh sized silica gel) using 25% ethyl acetate in petroleum ether to obtain as a yellow gummy liquid. Yield: 0.572 g, 50 %. IR ( $\nu$  cm<sup>-1</sup>, in KBr): 2981, 1249, 1024, 958. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.37-8.39 (m, 2H), 7.85-7.88 (m, 2H), 7.75 (dd, *J* = 1.9, 0.8 Hz, 1H), 7.54-7.58 (m, 2H), 7.46 – 7.42 (m, 2H), 6.65-6.66 (m, 1H), 6.71-6.72 (m, 1H), 4.28 (d, *J* = 22.7 Hz, 2H), 4.00 – 3.80 (m, 4H), 1.11 (t, *J* = 7.1 Hz, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 150.6, 142.9, 131.6 (d, *J* = 4.3 Hz), 130.1 (d, *J* = 6.7 Hz), 127.0, 126.3 (d, *J* = 6.2 Hz), 126.1, 126.0, 125.7 (d, *J* = 9.4 Hz), 125.2 (d, *J* = 3.0 Hz), 112.4, 110.9, 62.3 (d, *J* = 6.8 Hz), 27.5 (d, *J* = 140.7 Hz), 16.3 (d, *J* = 6.0 Hz). <sup>31</sup>P NMR (162 MHz, CDCl<sub>3</sub>) δ 25.3.



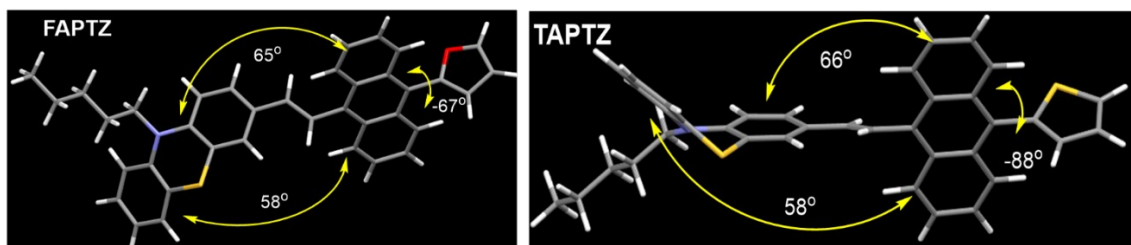
**Scheme S1:** Synthetic route for phosphonates



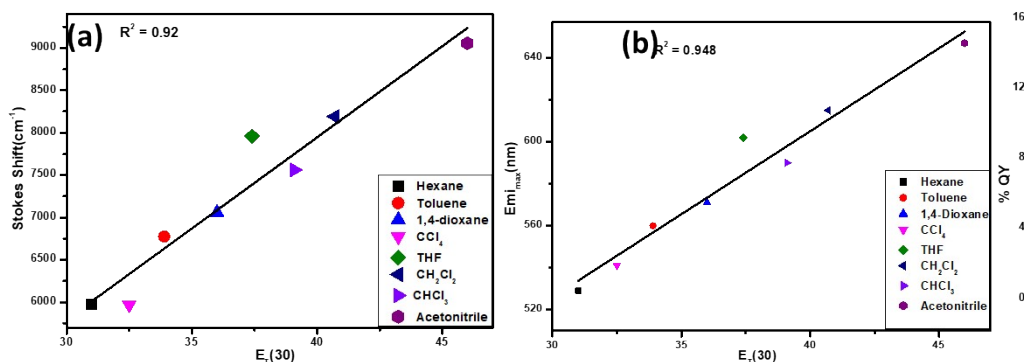
**Figure S1:** TGA plot for TAPTZ and FAPTZ



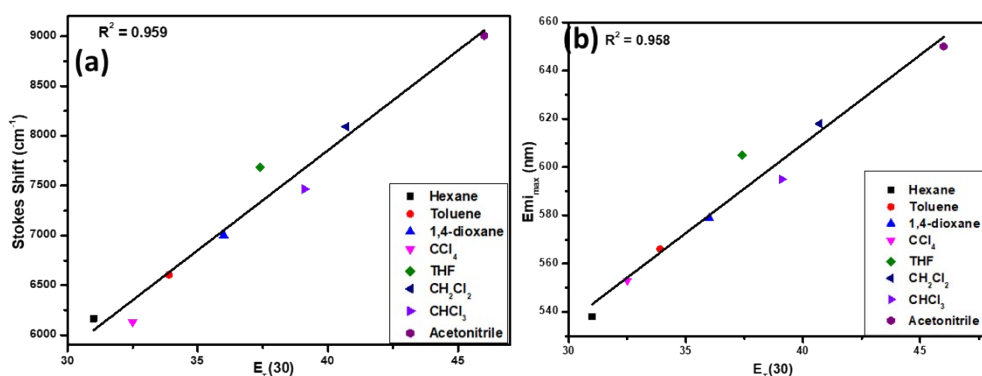
**Figure S2:** Absorbance and emission spectra of both spectra of both the compounds in different polar solvents.



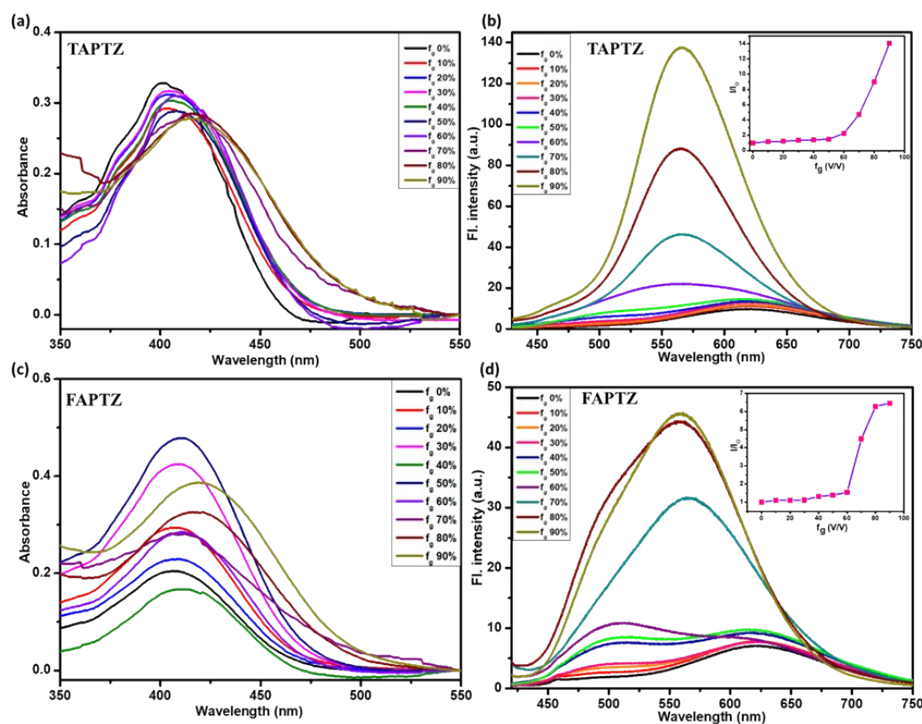
**Figure S3:** DFT-optimized (CAMB3LYP 6-31 G (d,p) Molecular structures



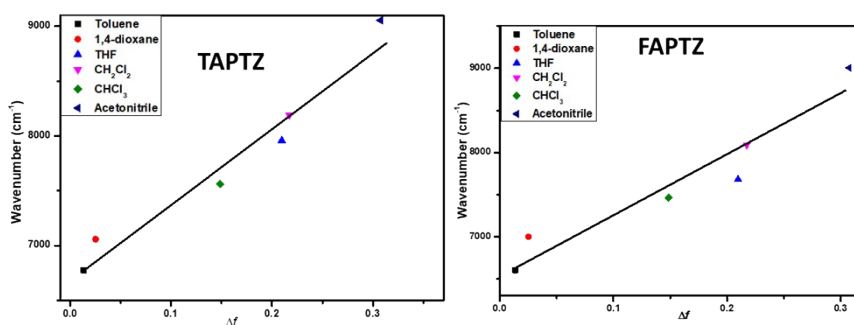
**Figure S4:** Compound TAPTZ; the plot of  $E_T(30)$  vs . (a) Stokes shift and (b) Emission max ( $\lambda_{\text{max}}$ )



**Figure S5:** Compound FAPTZ; the plot of  $E_T(30)$  vs . (a) Stokes shift and (b) Emission max ( $\lambda_{\text{max}}$ ).



**Figure S6:** Compound TAPTZ and FAPTZ ( $10^{-5}$  M) with different fraction of glycerol in MeOH showing viscochromism (a) Absorption Spectra of TAPTZ (b) Emission spectra of TAPTZ. (c) Absorption Spectra of FAPTZ (d) Emission spectra of FAPTZ. ( $\lambda_{\text{ex}} = 405$  nm)



**Figure S7:** Lippert-Mataga Plot ( $\Delta f$  vs Stokes shift in different solvents)

The difference in dipole moment between ground and singlet excited state was calculated using the formula

$$m = \frac{2(\mu_e - \mu_g)^2}{hca^3}$$

The slopes  $m$  was obtained from the Lippert–Mataga plots.

For **FAPTZ**

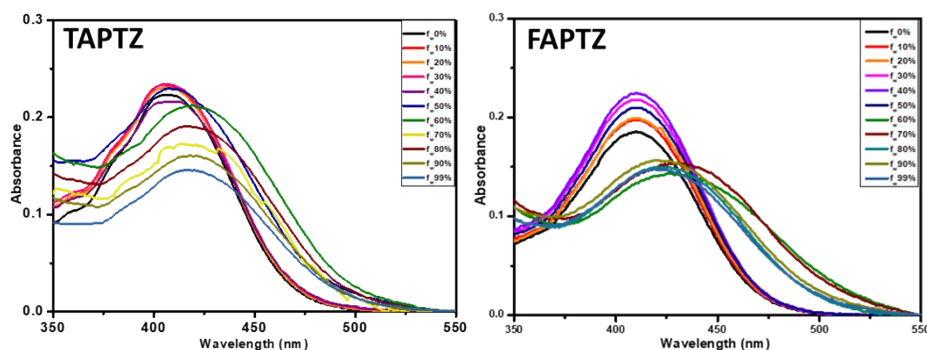
$$a = 6.529 \text{ \AA} ; \text{slope}(m) = 7004.14$$

For **TAPTZ**

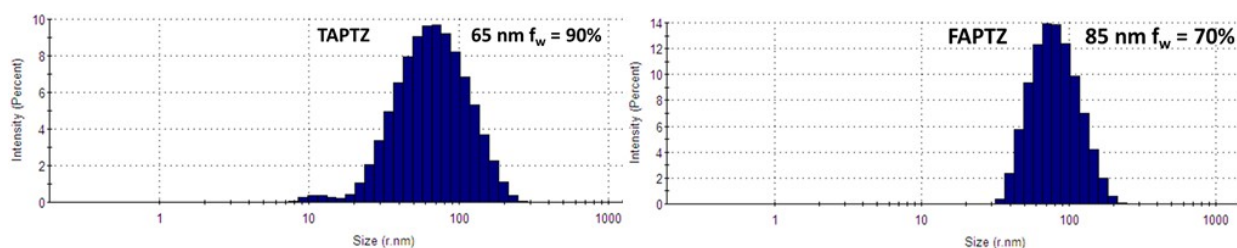
$$a = 6.68 \text{ \AA} ; \text{slope}(m) = 6970.7$$

**Table S1:** Shift and the difference between excited and ground state dipole moment

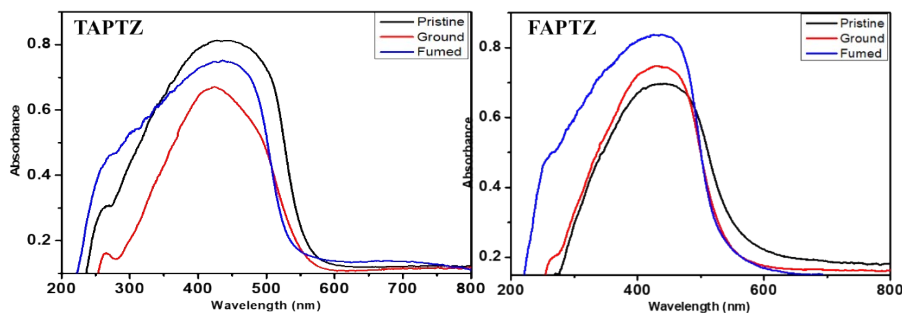
Compounds	Emission $\lambda_{\max}$ (nm) (Hexane)	Emission $\lambda_{\max}$ (nm) (MeCN)	Emission $\Delta\lambda_{\max}$ (nm)	Shift type	Difference in dipole moment ( $\mu_e - \mu_g$ )
<b>TAPTZ</b>	528	646	118	Red	14.37 D
<b>FAPTZ</b>	537	644	107	Red	13.91 D



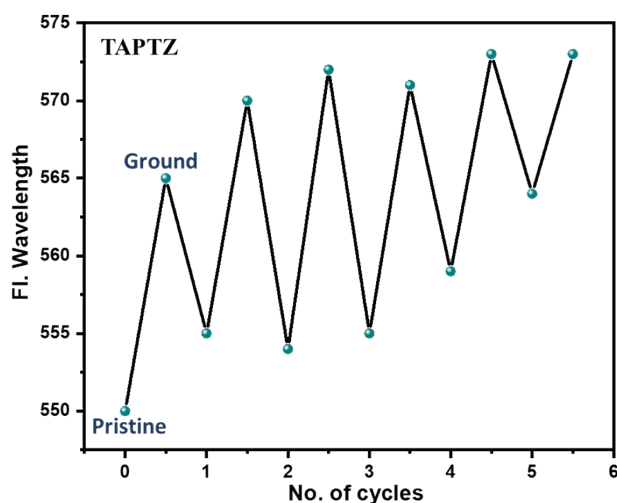
**Figure S8:** UV-vis spectra with different fraction of H<sub>2</sub>O in MeCN



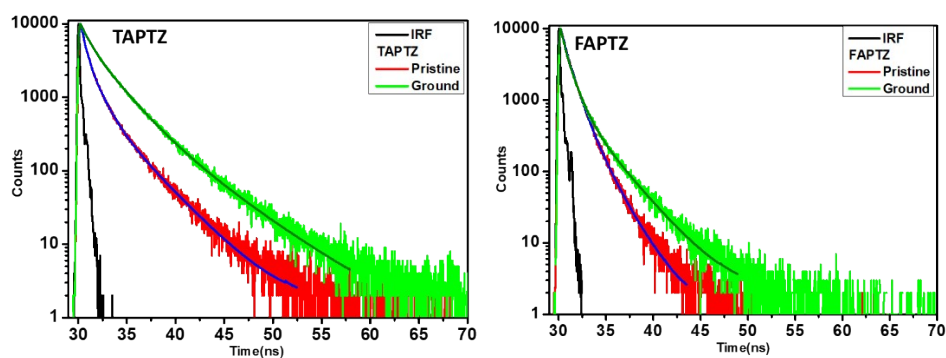
**Figure S9:** DLS studies of the compounds



**Figure S10:** Solid-state absorption spectra for TAPTZ and FAPTZ before and after grinding



**Figure S11:** The plot of maximum emission wavelength changes with multiple grinding/Fuming process.



**Figure S12:** Solid-state lifetime decay for TAPTZ and FAPTZ

**Table S2:** Parameter related to lifetime ( $\tau$ ; ns) measurement of excited state.  $\lambda_{\text{ex}} = 405 \text{ nm}$ 

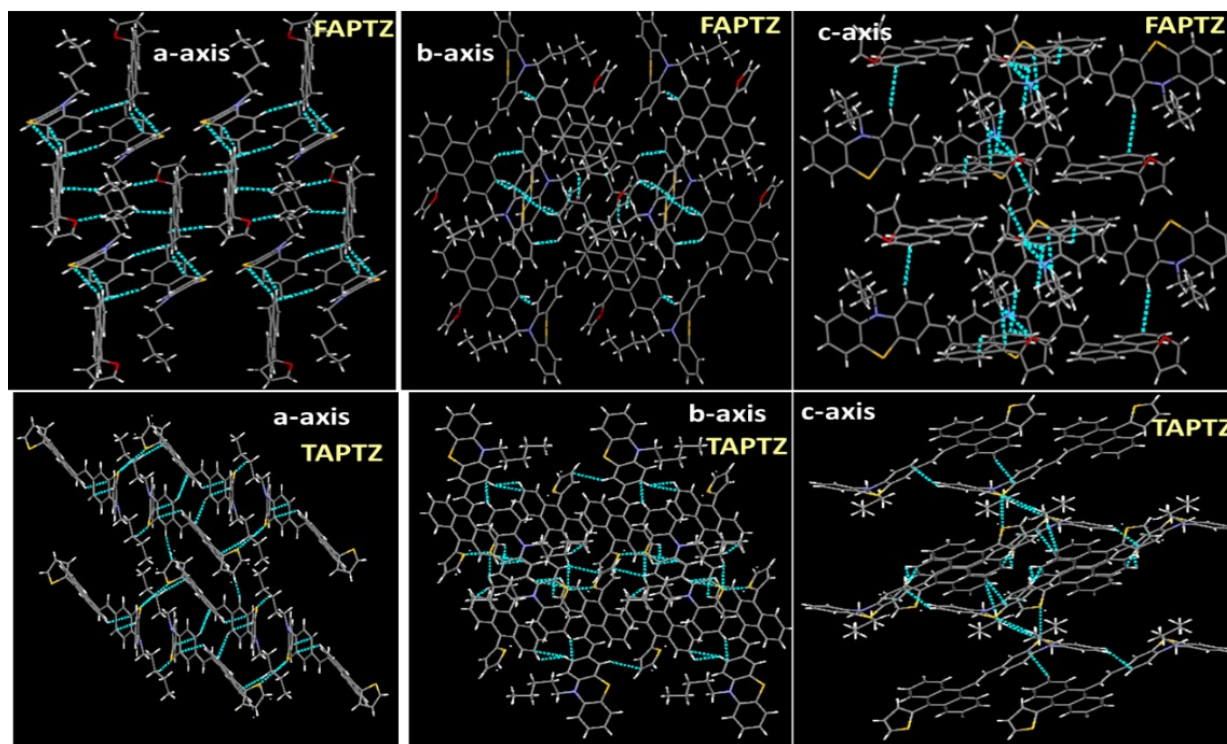
Compounds	States	$\alpha_1$	$\alpha_2$	$\alpha_3$	$\alpha_4$	$\tau_1$	$\tau_2$	$\tau_3$	$\tau_4$	$\langle\tau\rangle$	$\chi^2$
<b>TAPTZ</b>	Pristine	0.24	0.05	0.70		1.11	3.19	0.29		0.65	1.05
	Ground	0.27	0.29	0.05	0.38	0.61	2.33	4.88	0.11	1.16	1.06
<b>FAPTZ</b>	Pristine	0.34	0.07	0.58	0.88	1.88	0.24	0.57	1.27	0.57	1.27
	Ground	0.25	0.05	0.7	0.95	2.83	0.23	0.54	1.22	0.54	1.22

**Table S3.** Single-crystal X-ray table

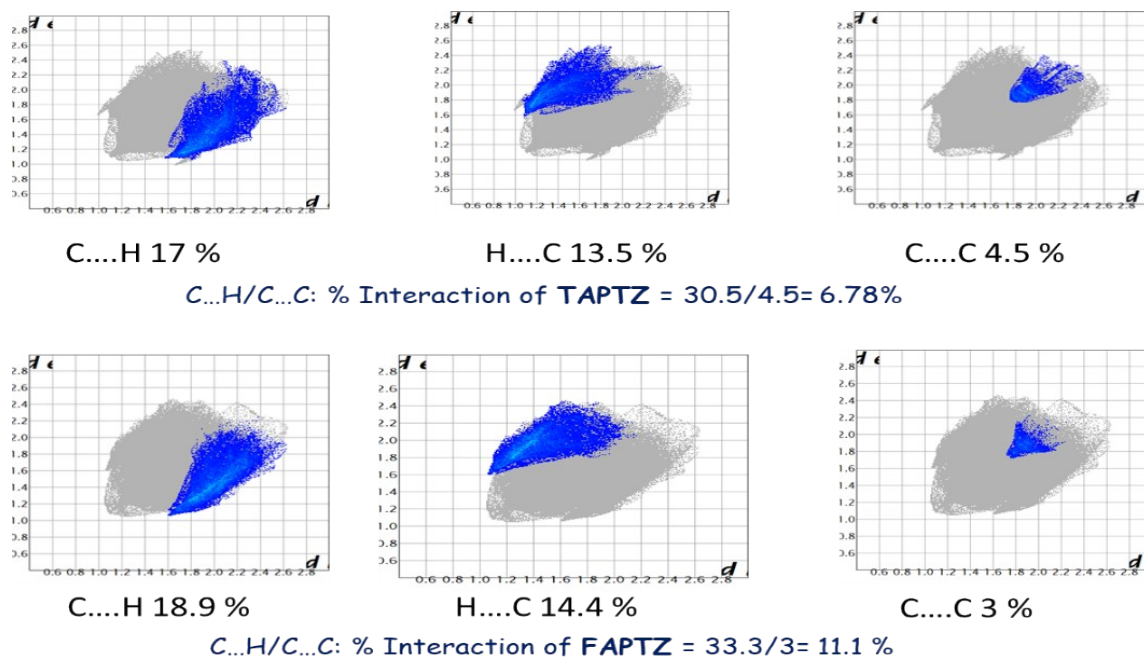
Compounds	TAPTZ	FAPTZ
Emp. Formula	$\text{C}_{37}\text{H}_{31}\text{NS}_2$	$\text{C}_{37}\text{H}_{31}\text{NOS}$
Formula Weight	553.78	537.72
Crystal System	Triclinic	Triclinic
Space Group	P-1	P-1
a /Å	9.7359	9.4072
b /Å	11.8665	12.0367
c /Å	13.2451	12.9302
$\alpha$ /degree	79.713	75.199
$\beta$ /degree	69.428	75.683
$\gamma$ /degree	88.969	81.825
V /Å <sup>3</sup>	1407.95(2)	1366.68(4)
Z	2	2
D <sub>calc</sub> /g cm <sup>-3</sup>	1.306	1.307
$\mu$ /mm <sup>-1</sup>	1.912	1.287
F (000)	584	568
Data/ restraints/ parameters	5893/12/394	5734/0/362
S	1.078	1.011
R1 [ $I > 2\sigma(I)$ ]	0.0358	0.048
wR2 [all data]	0.0989	0.1322



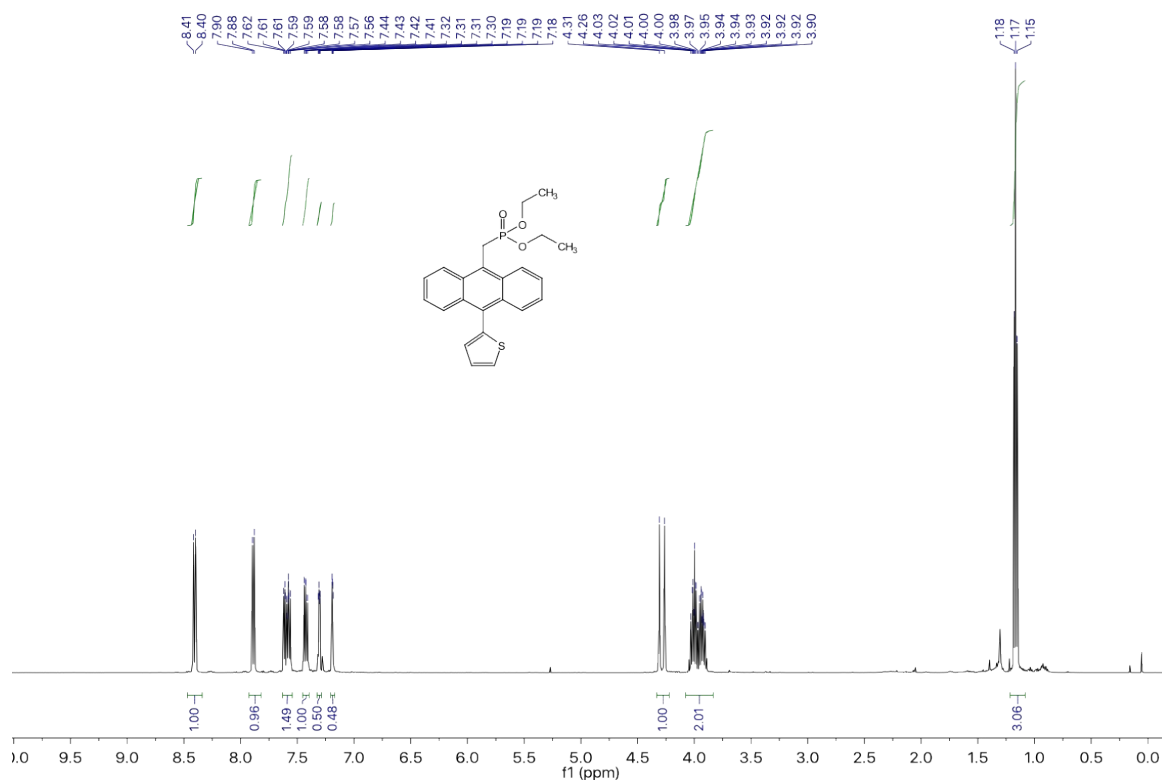
Max./min. residual electron dens. [eÅ <sup>-3</sup> ]	0.243/-0.335	0.5125/-0.5248
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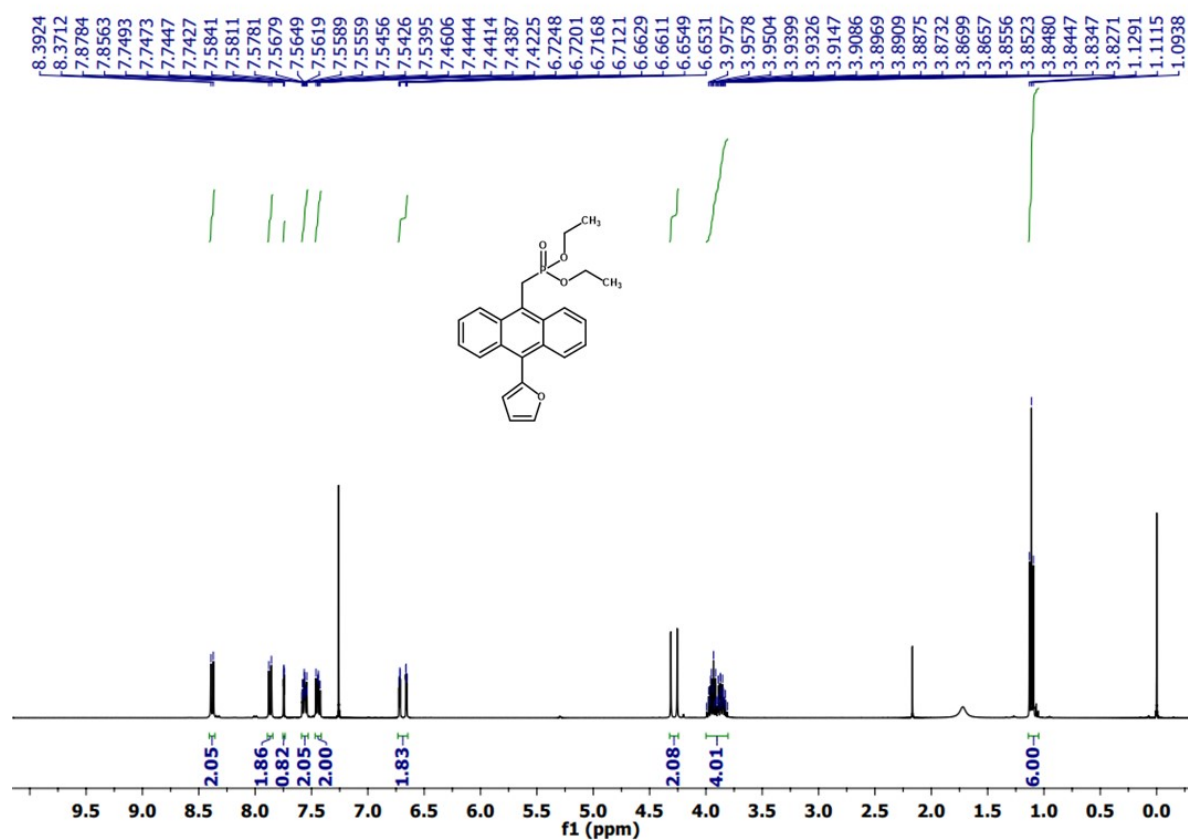
**Figure S13:** Crystal packing diagram from all the axes



**Figure S14:**  $d_{\text{norm}}$  Hirshfeld surfaces for TAPTZ and FAPTZ and their 2D finger plots of C...H, H...C and C...C interactions,



**Figure S15:**  $^1\text{H-NMR}$  spectrum of Thiophene linked anthracenyl phosphonate in  $\text{CDCl}_3$



**Figure S16:**  $^1\text{H-NMR}$  spectrum of Furan linked anthracenyl phosphonate in  $\text{CDCl}_3$

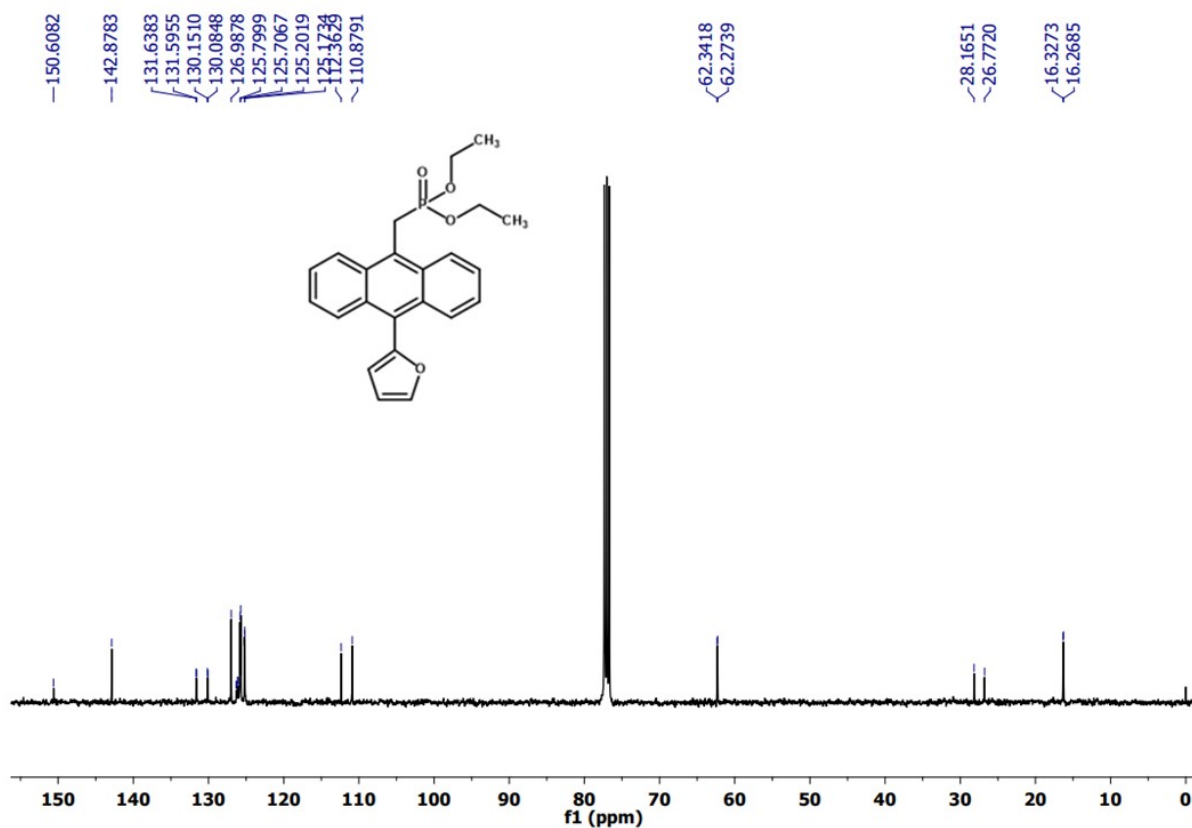


Figure S17: <sup>13</sup>C-NMR spectrum of Furan linked anthracenyl phosphonate in CDCl<sub>3</sub>

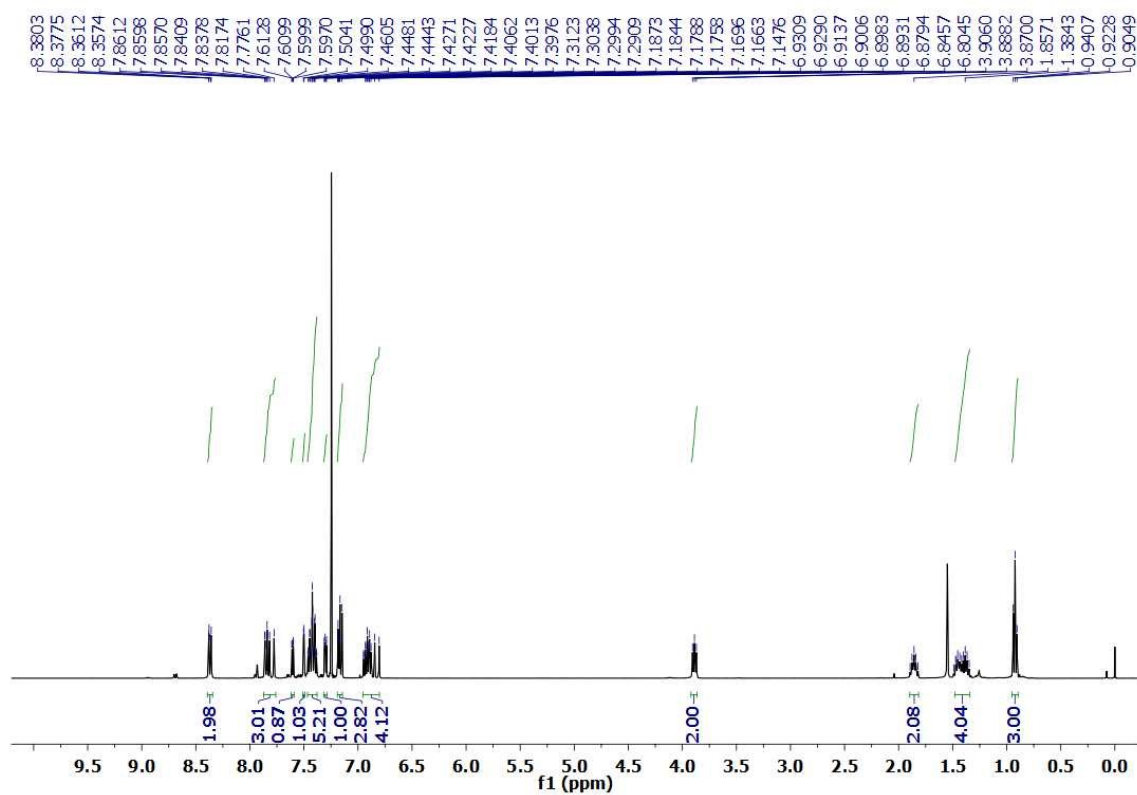


Figure S18: <sup>1</sup>H NMR spectrum for TAPTZ in CDCl<sub>3</sub>

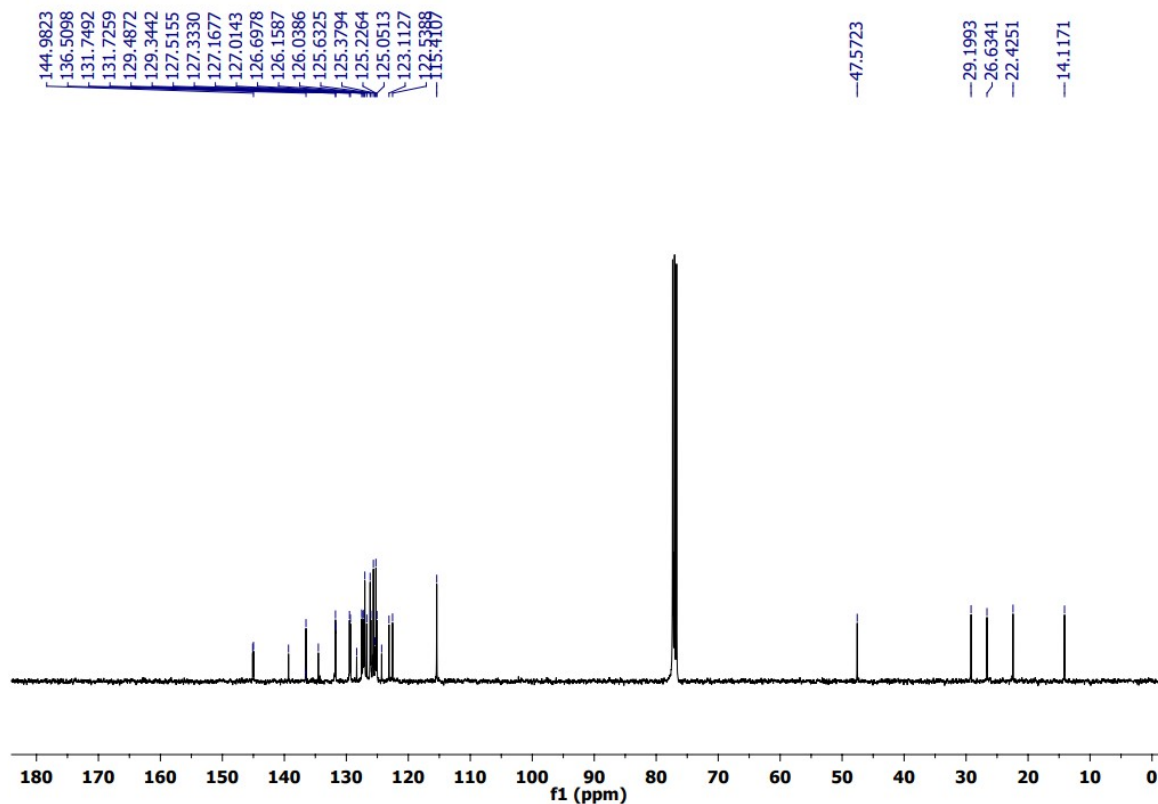


Figure S19:  $^{13}\text{C}$  NMR spectrum for TAPTZ in  $\text{CDCl}_3$

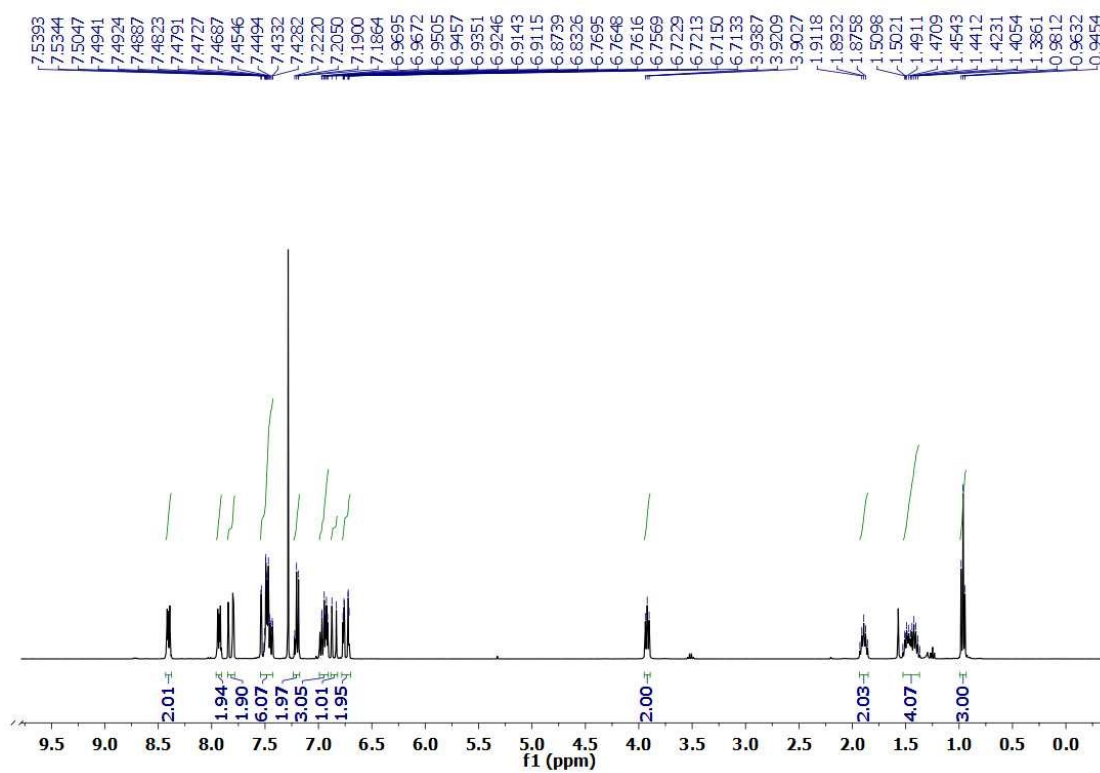
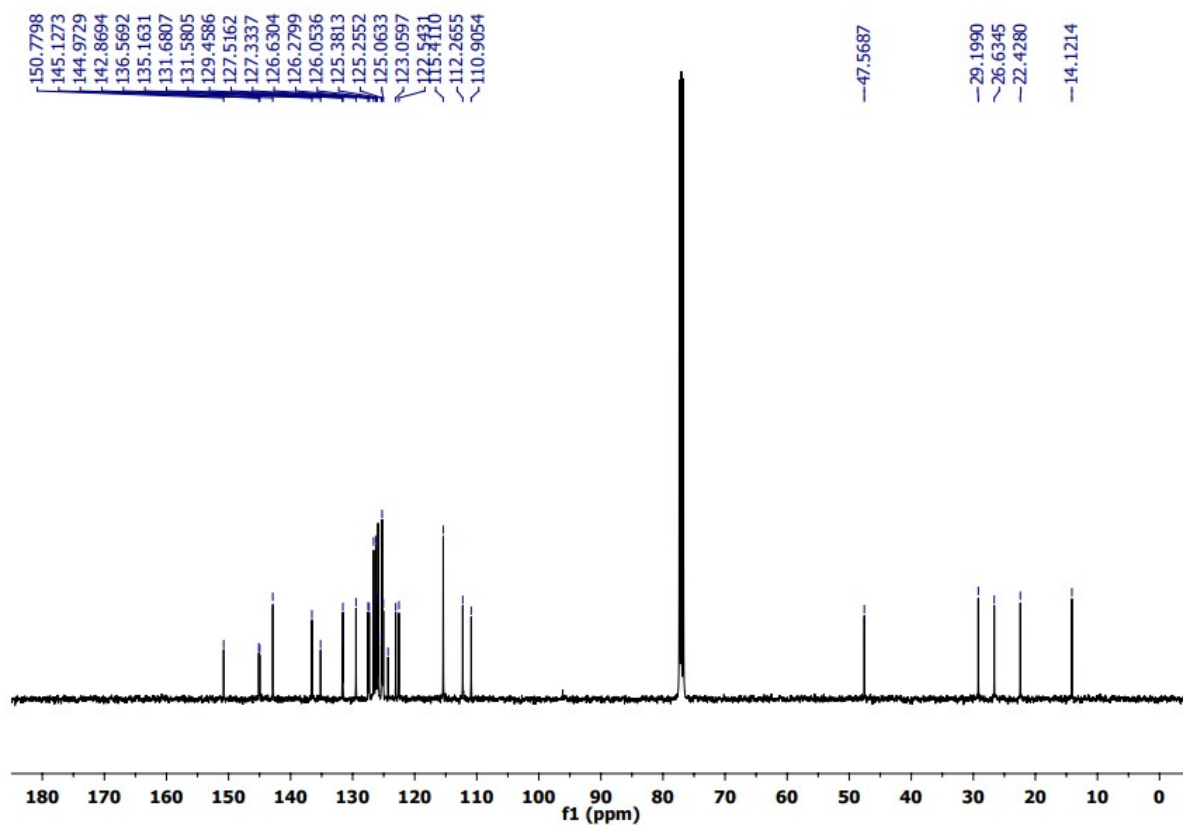


Figure S20:  $^1\text{H}$  NMR spectrum for FAPTZ in  $\text{CDCl}_3$



**Figure S21:**  $^{13}\text{C}$  NMR spectrum for **FAPTZ** in  $\text{CDCl}_3$

### References

1. M. Z. K. Baig, G. Pallikonda, P. Trivedi, R. N. P. Tulichala, B. Ghosh and M. Chakravarty, *ChemistrySelect*, 2016, **1**, 4332–4339.

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