Supporting Informations

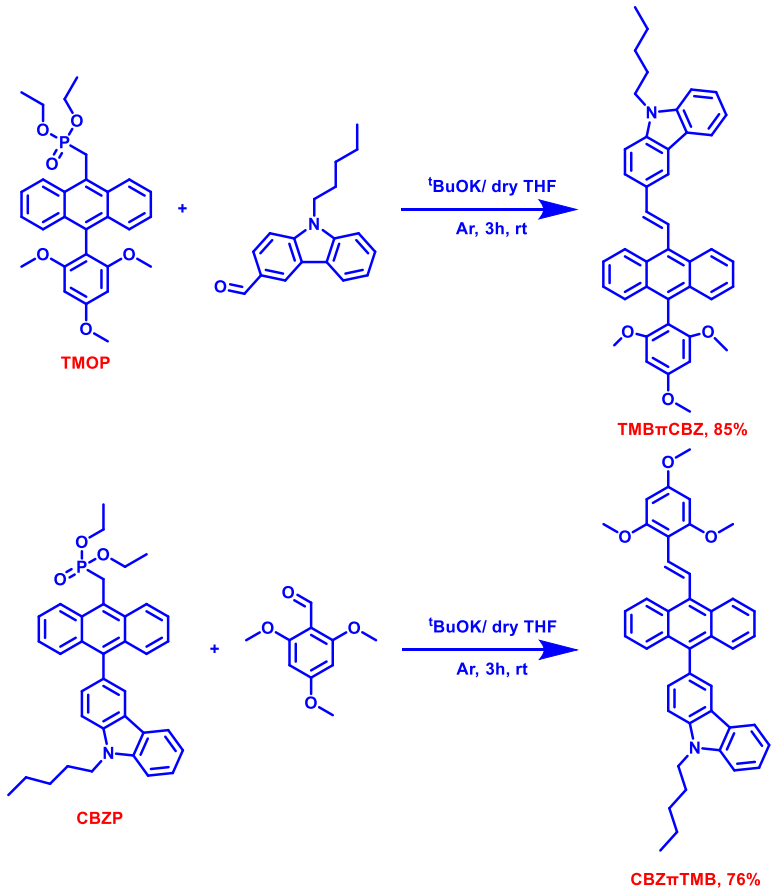
For

The disparity in piezofluorochromism for twisted mono-carbazole-based AIEgens by interchanging electron-rich substituents: Effect of coplanarity on twisted π-conjugates

Banchhanidhi Prusti and Manab Chakravarty*

Department of Chemistry, BITS-Pilani Hyderabad Campus, Jawahar Nagar, Shameerpet, Hyderabad-500078, Telangana (India)

Contents:



Scheme S1: Synthetic route for **TMBπCBZ** and **CBZπTMB**

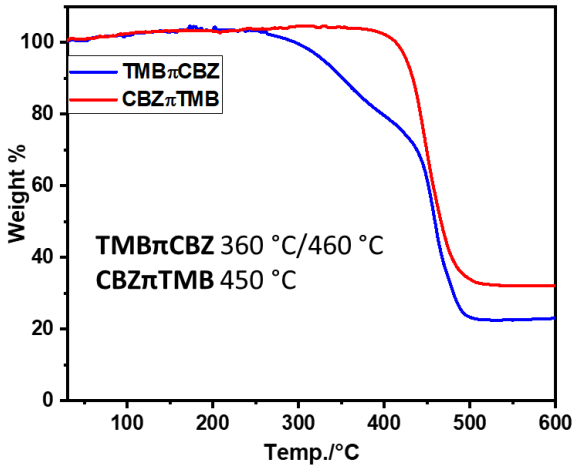


Fig S1: TGA plot for **TMBπCBZ** and **CBZπTMB**

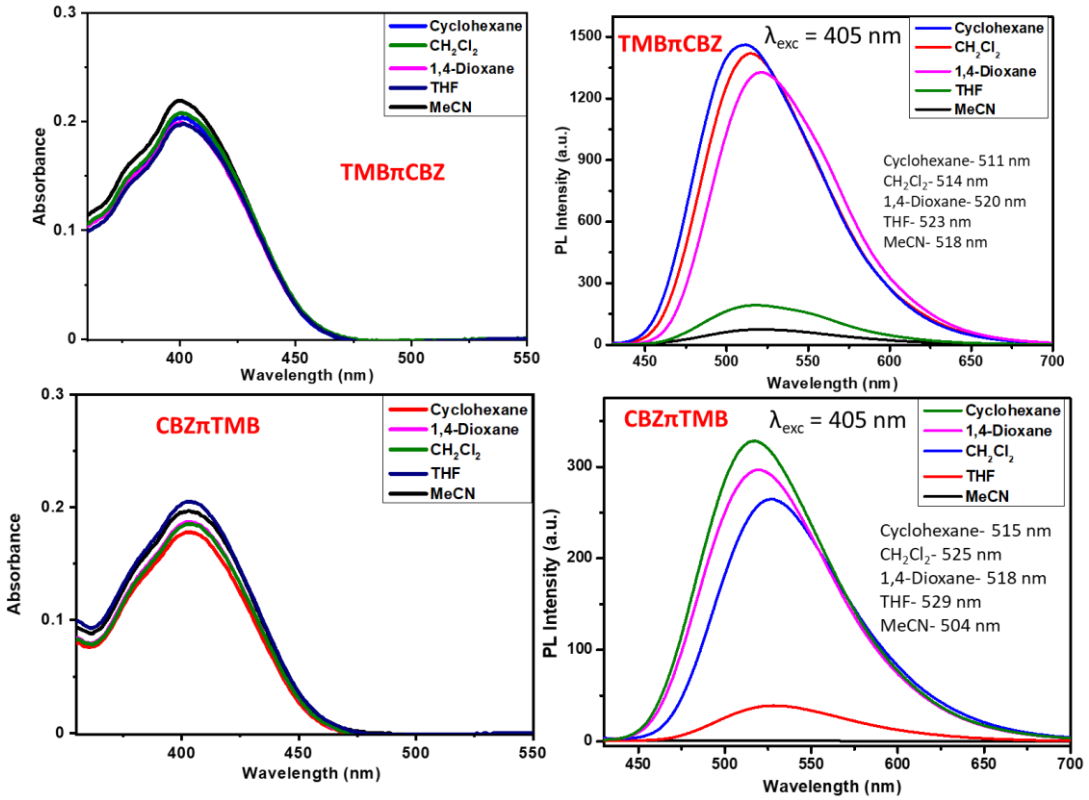


Fig S2: Absorbance and emission spectra of both the positional isomers in different polar solvents.

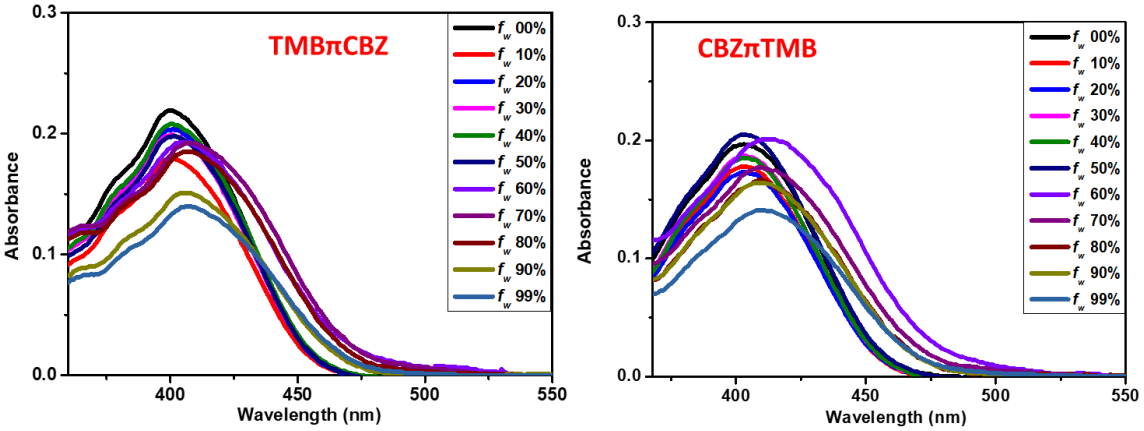


Fig S3: Absorption spectra of the compounds. 10 µM acetonitrile solution upon gradual addition of water fraction [a nonsolvent f_w (v/v%)]

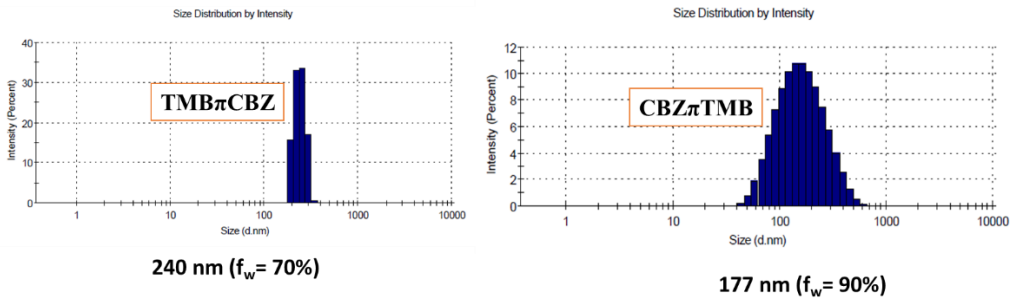


Fig S4: DLS studies for **TMBπCBZ** and **CBZπTMB** at f_w= 70% and f_w= 90% respectively.

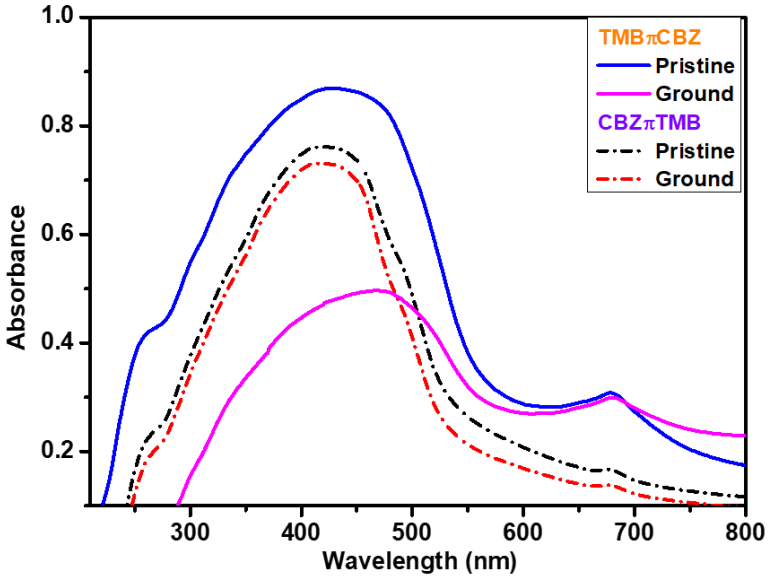


Fig S5: solid-state absorption spectra for **TMBπCBZ** and **CBZπTMB** before and after grinding

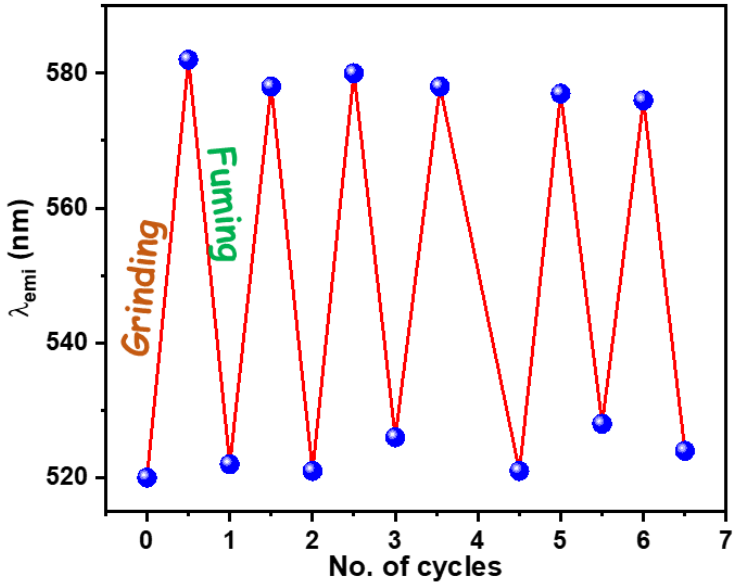


Fig S6: The plot of maximum emission wavelength changes with multiple grinding/Fuming process.

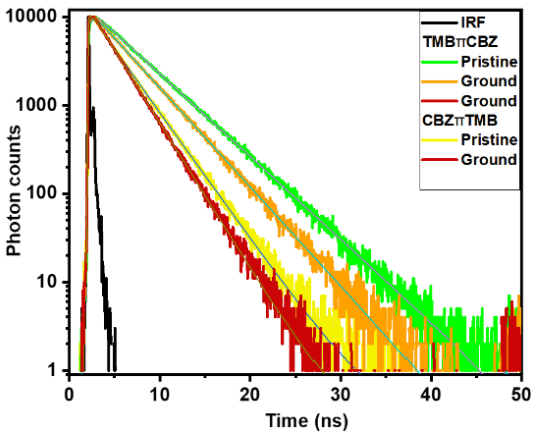


Fig S7: Solid-state lifetime decay for **TMBπCBZ** and **CBZπTMB**

Table S1: Parameter related to lifetime measurement of excited state.

Samples	States	α_1	α_2	T_1	T_2	χ^2	τ (ns)
TMBπCBZ	Pristine	0.07	0.93	0.03	4.35	1.09	4.05
	Ground	0.12	0.88	0.3	2.64	1.01	2.36
CBZπTMB	Pristine	0.28	0.72	0.45	2.9	1.21	2.21
	Ground	0.32	0.68	0.85	1.8	1.11	1.50

Table S2. Single-crystal X-ray table for **TMBπCBZ** and **CBZπTMB**

Compounds	**TMBπCBZ**	**CBZπTMB**
Emp. Formula	C42 H39 N O3	C42 H39 N O3
Formula weight	605.74	605.74
Crystal system	triclinic	monoclinic
Space group	P -1	P 1 21/n 1
a /Å	8.9859(3)	8.89830(10)
b /Å	12.6291(2)	14.1159(4)
c /Å	15.4962(4)	25.3397(3)

α/degree	72.582(2)	90
β/degree	77.414(2)	93.5670(10)
γ/degree	80.067(2)	90
V /Å^3	1626.71(8)	3176.69(10)
Z	2	4
D_{calc} /g cm^{-3}]	1.265	1.267
μ /mm^{-1}	0.612	0.615
F (000)	660.0	1288.0
Data/ restraints/ parameters	6246 /0/429	5598/0/419
S	1.056	1.035
R1 [I>2σ(I)]	0.0396	0.0501
wR2 [all data]	0.1116	0.1438
Max./min. residual electron dens. [eÅ^{-3}]	0.327/-0.238	0.326/-0.263

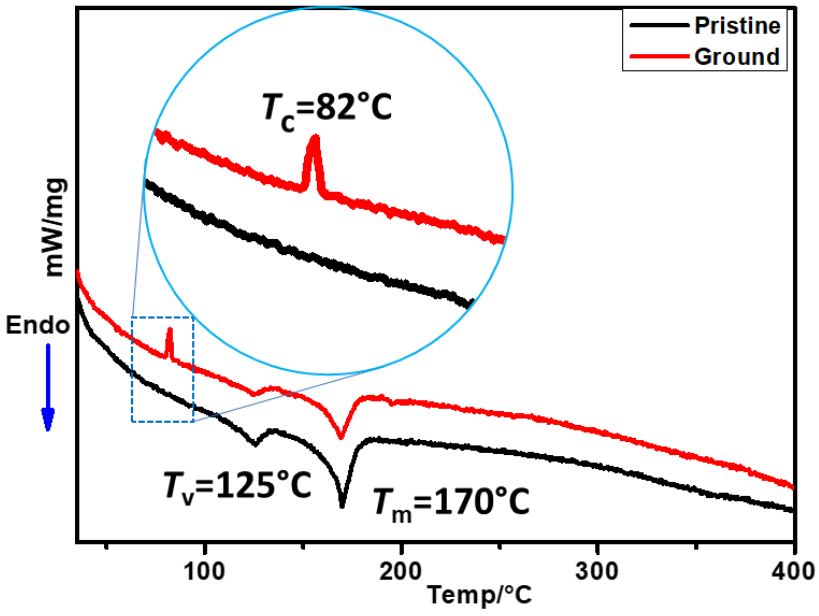


Fig S8: DSC thermogram for PFC-active **TMBπCBZ** in pristine and ground state.

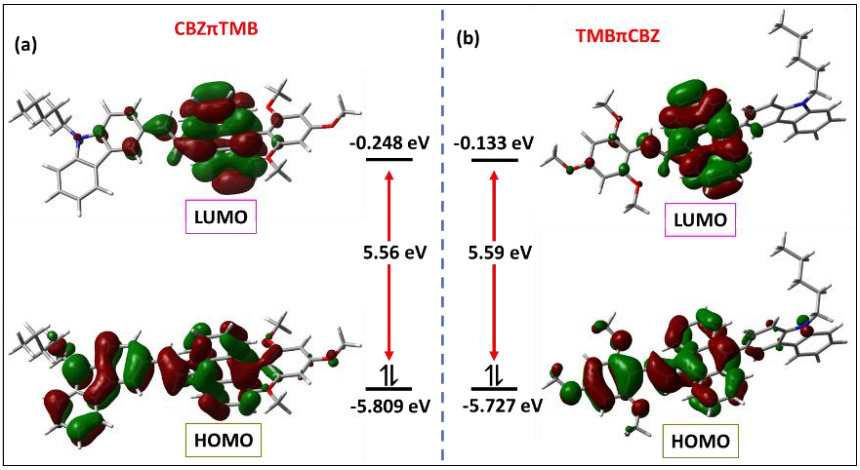


Fig S9: Molecular Orbital diagram for **TMBπCBZ** and **CBZπTMB**

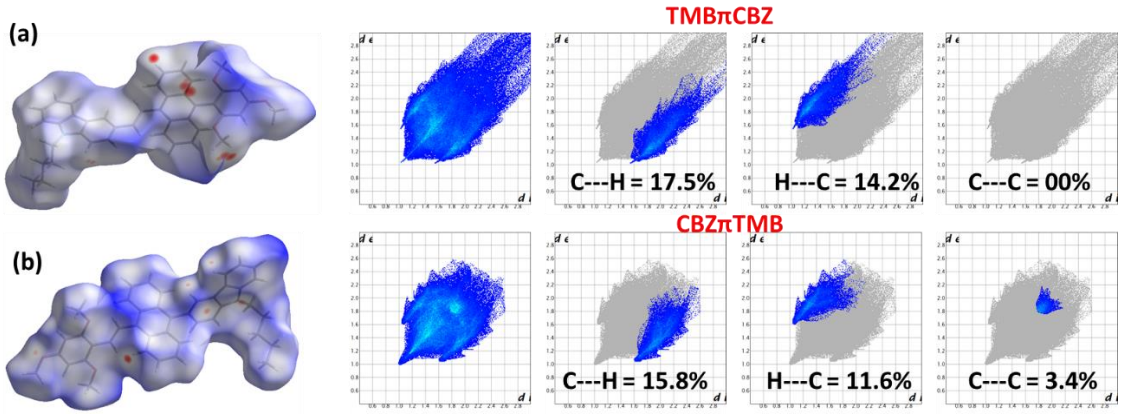


Fig S10: (a) d_{norm} Hirshfeld surface for **TMBπCBZ** and their 2D finger plots of C…H, H…C and C…C interactions, (b) d_{norm} Hirshfeld surface for **CBZπTMB** and their 2D finger plots of C…H, H…C and C…C interactions

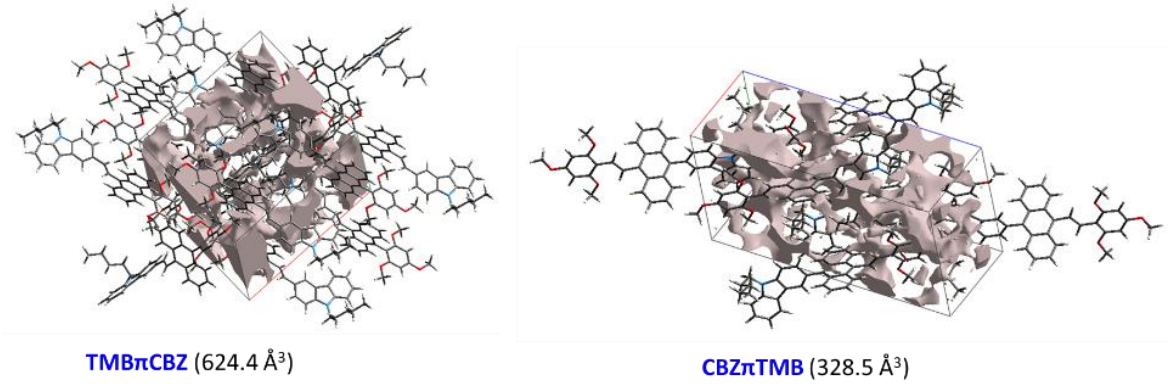


Fig S11: Void space for the isomers calculated from crystal Explorer 17.

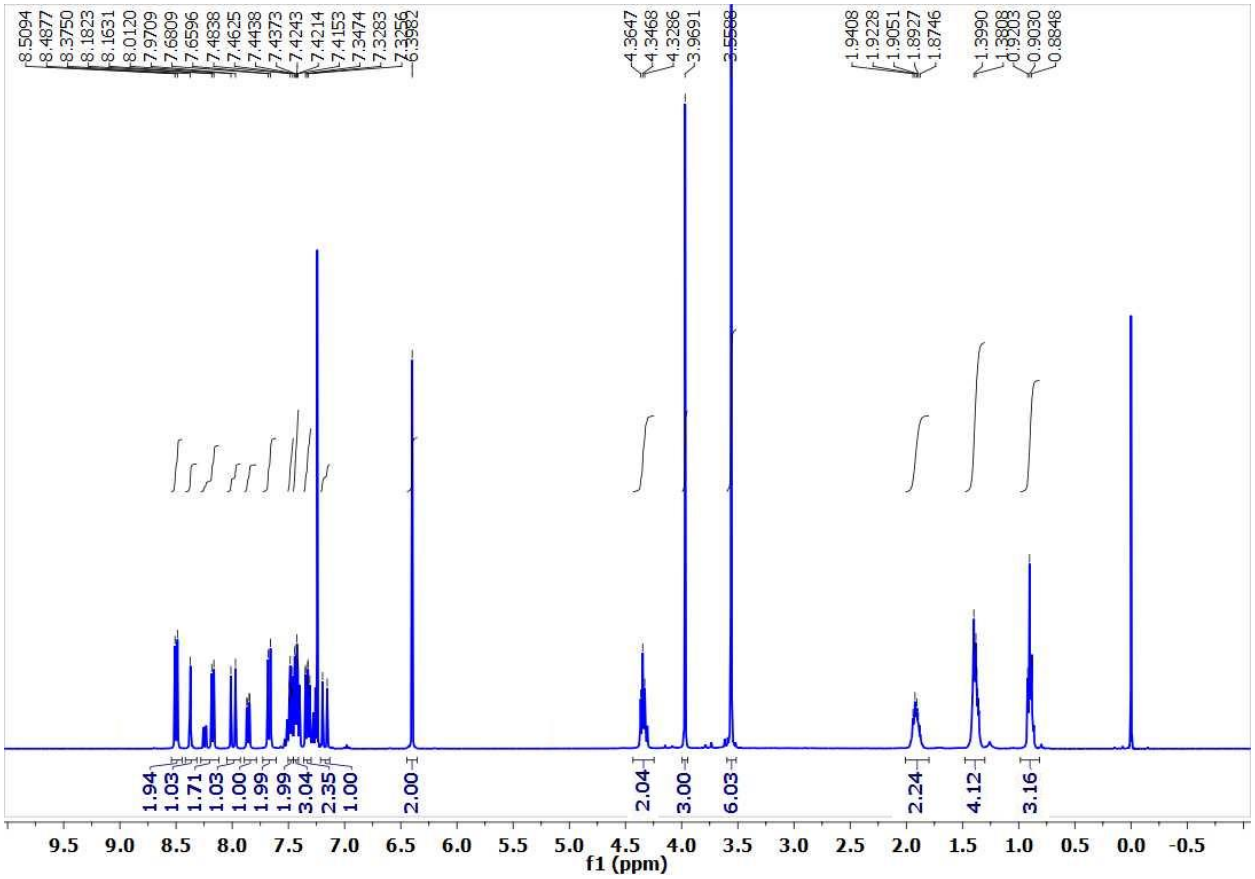


Fig S12: ^{1}H NMR spectrum for **TMBπCBZ** in $CDCl_3$

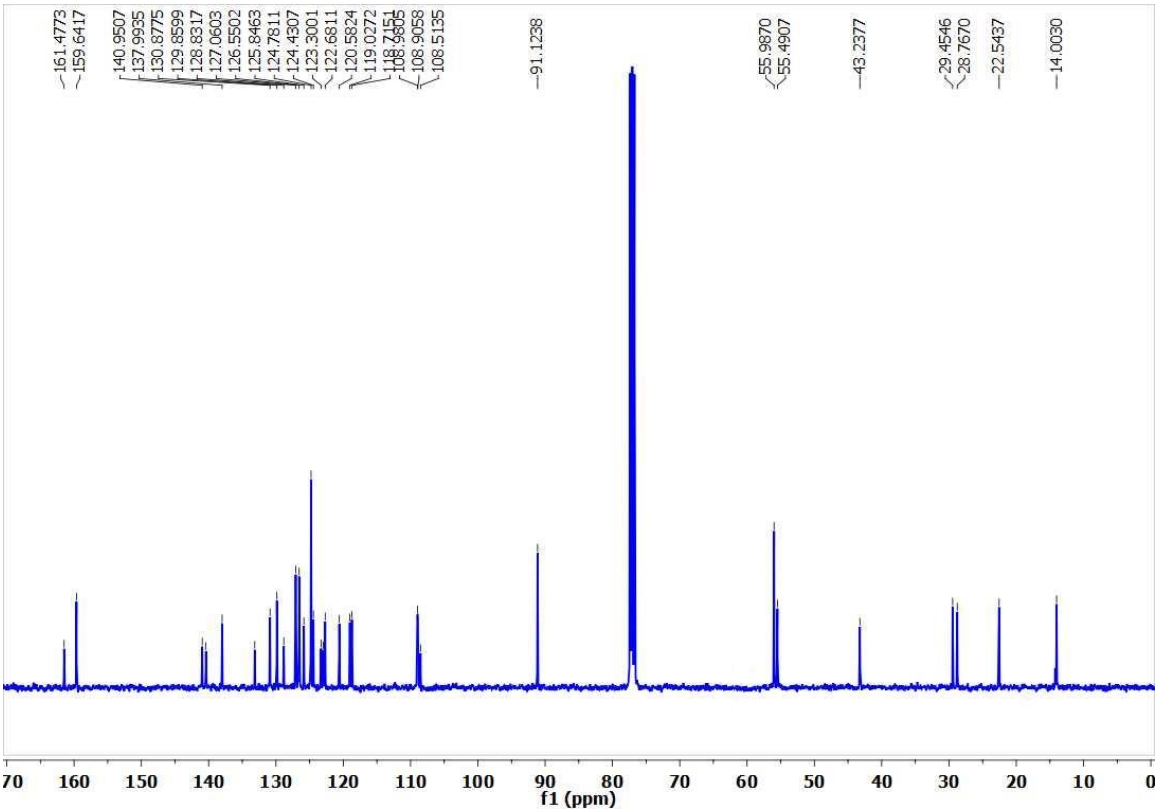


Fig S13: ^{13}C NMR spectrum for **TMBπCBZ** in $CDCl_3$

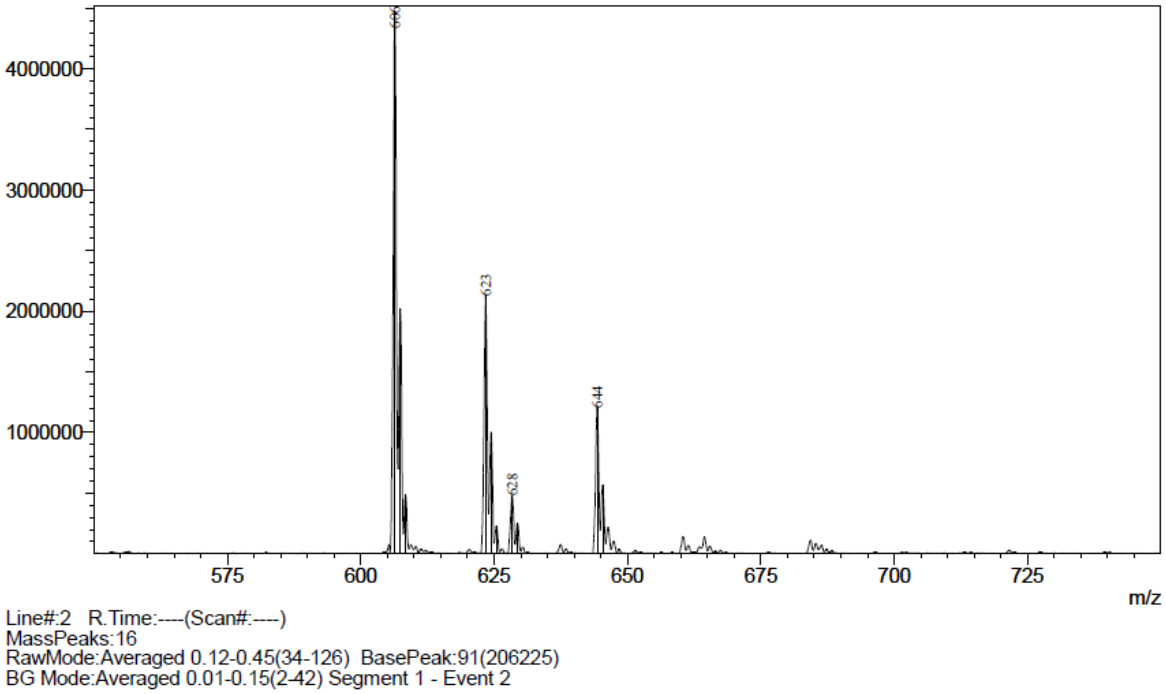


Fig S14: ESI-MS spectrum for **TMBπCBZ**

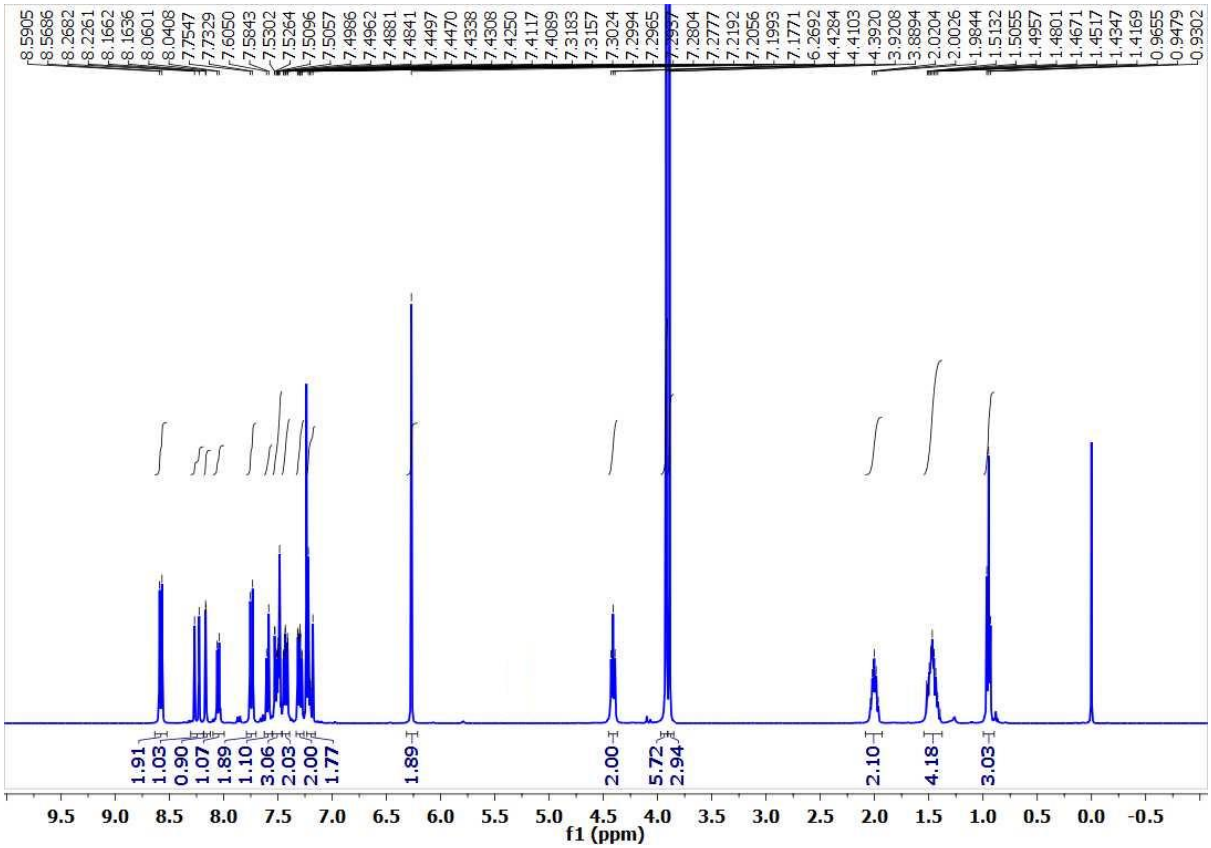


Fig S15: ^{1}H NMR spectrum for **CBZπTMB** in $CDCl_3$

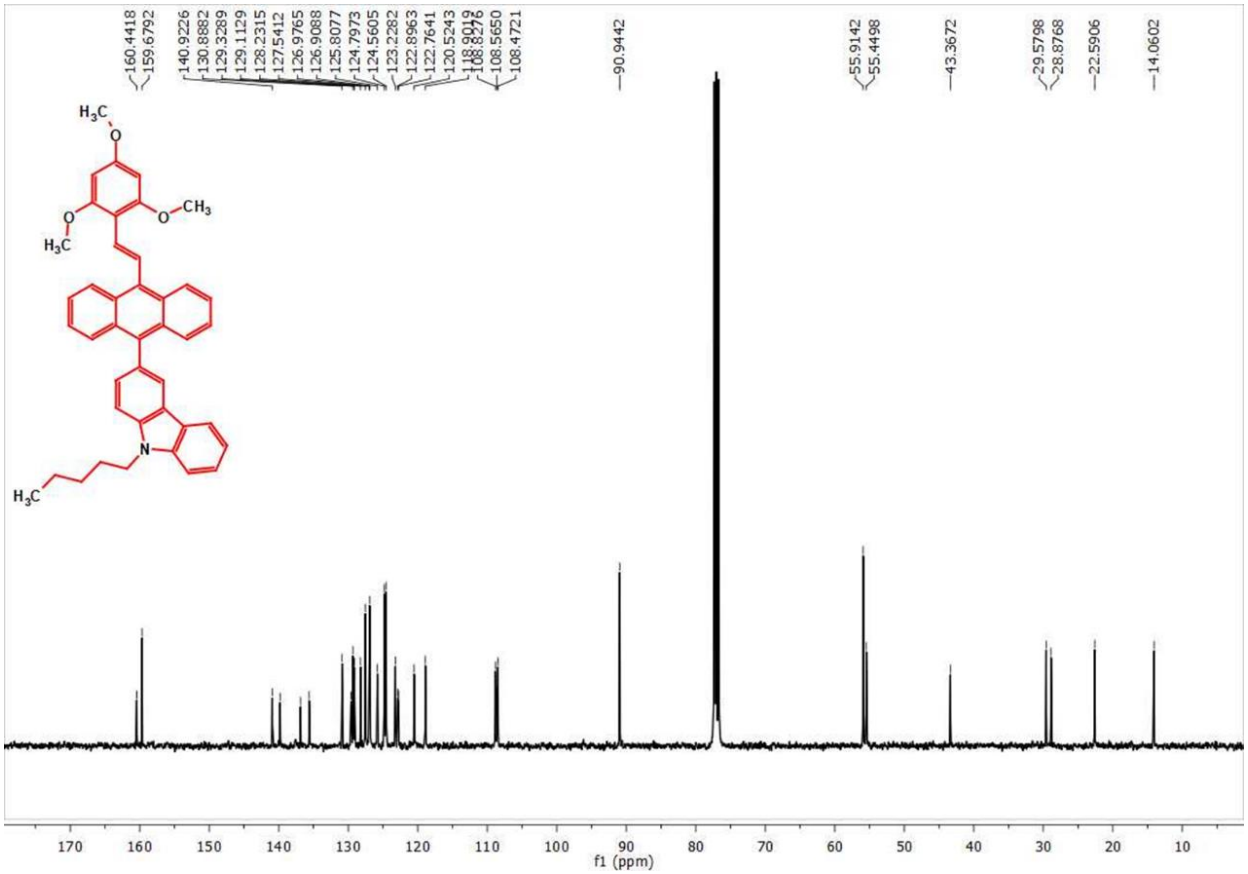


Fig S16: ^{13}C NMR spectrum for **CBZπTMB** in $CDCl_3$

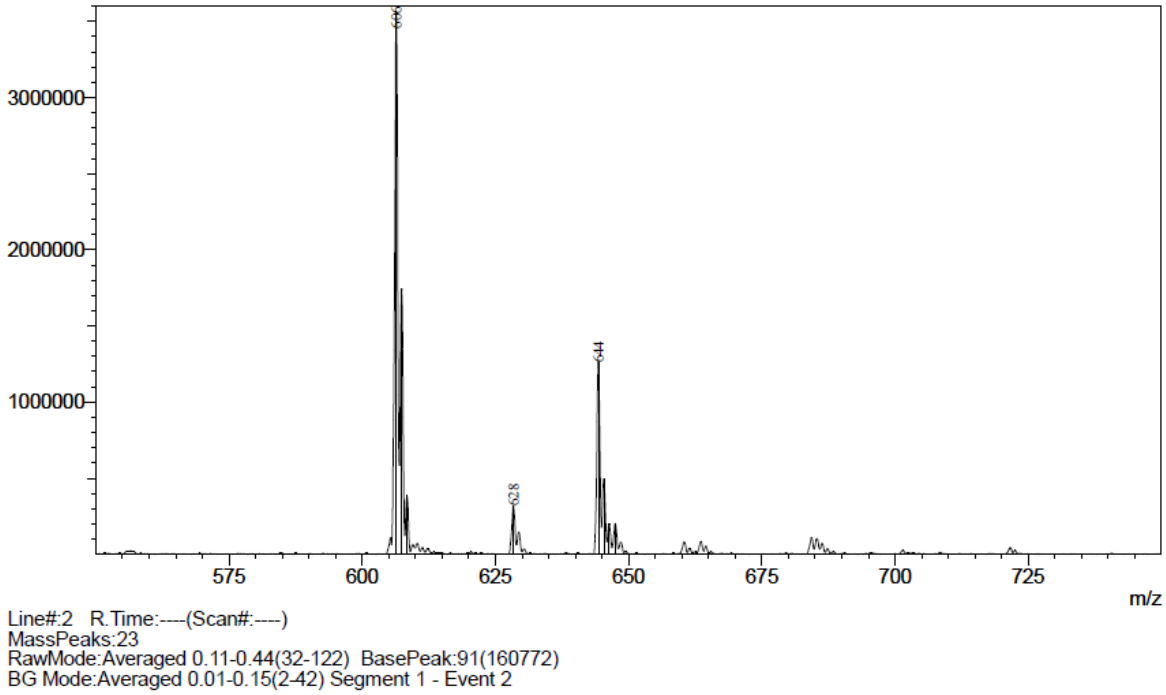


Fig S17: ESI-MS spectrum for **CBZπTMB**

END