

Supporting Informations

For

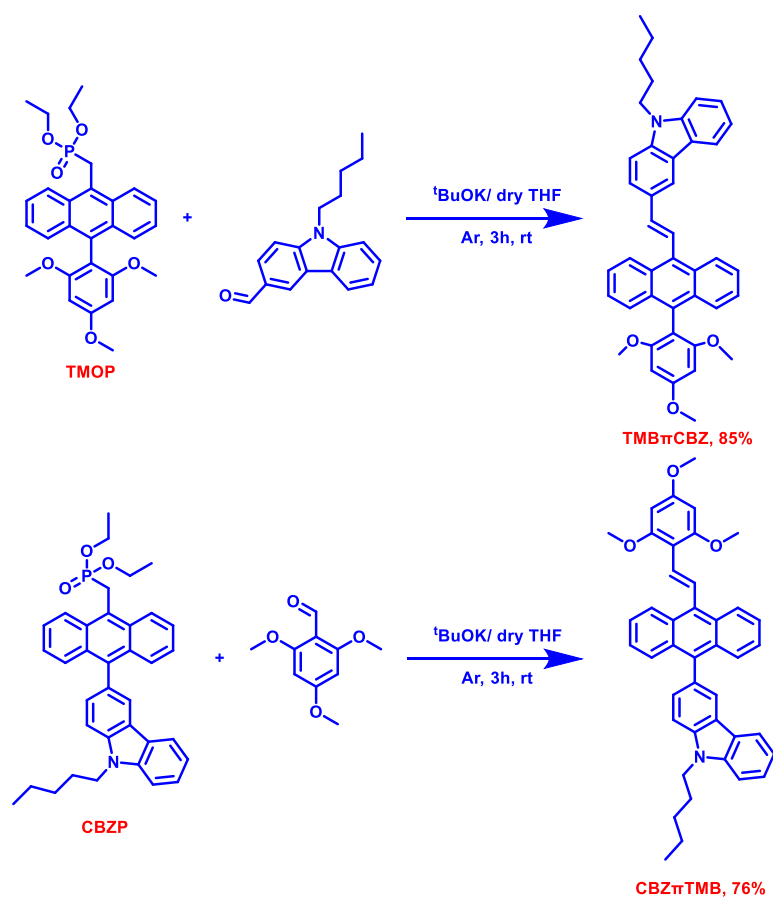
The disparity in piezofluorochromism for twisted mono-carbazole-based AIEgens by interchanging electron-rich substituents: Effect of coplanarity on twisted π -conjugates

Banchhanidhi Prusti and Manab Chakravarty*

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

Contents:

1. Synthetic scheme for TMB π CBZ and CBZ π TMB (Scheme-1)	S2
2. Thermogravimetric analysis (TGA) plot (Fig-S1)	S2
3. Solution-state abs. and emission spectra (Fig-S2)	S3
4. Absorption spectra at different fractions of water (Fig-S3)	S3
5. Dynamic light scattering (DLS) plots (Fig-S4)	S3
6. Solid-state absorption spectra before and after grinding (Fig-S5)	S4
7. PFC emission wavelength for multiple grinding/fuming (Fig-S6)	S4
8. Solid-state lifetime decay plots (Fig-S7)	S5
9. Lifetime measurement table (Table-S1)	S5
10. Single-crystal X-ray table (Table-S1)	S5-S6
11. DSC plot before and after grinding for TMB π CBZ (Fig-S8)	S6
12. Molecular orbital diagram (Fig-S9)	S7
13. Hishfeld surface 2D fingerprint plots (Fig-S10)	S7
14. Void space diagram (Fig-S11)	S7
15. ^1H NMR spectra for TMB π CBZ (Fig-S12).....	S8
16. ^{13}C NMR spectra for TMB π CBZ (Fig-S13).....	S8
17. ESI-MS spectra for TMB π CBZ (Fig-S14).....	S9
18. ^1H NMR spectra for CBZ π TMB (Fig-S15).....	S9
19. ^{13}C NMR spectra for CBZ π TMB (Fig-S16).....	S10
20. ESI-MS spectra for TMB π CBZ (Fig-S17).....	S10



Scheme S1: Synthetic route for **TMB π CBZ** and **CBZ π TMB**

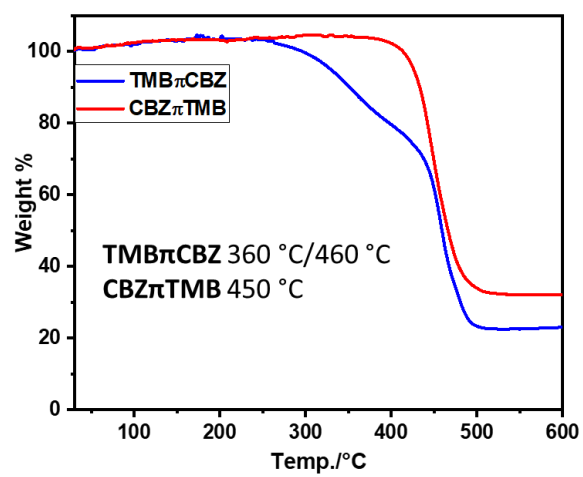


Fig S1: TGA plot for **TMB π CBZ** and **CBZ π TMB**

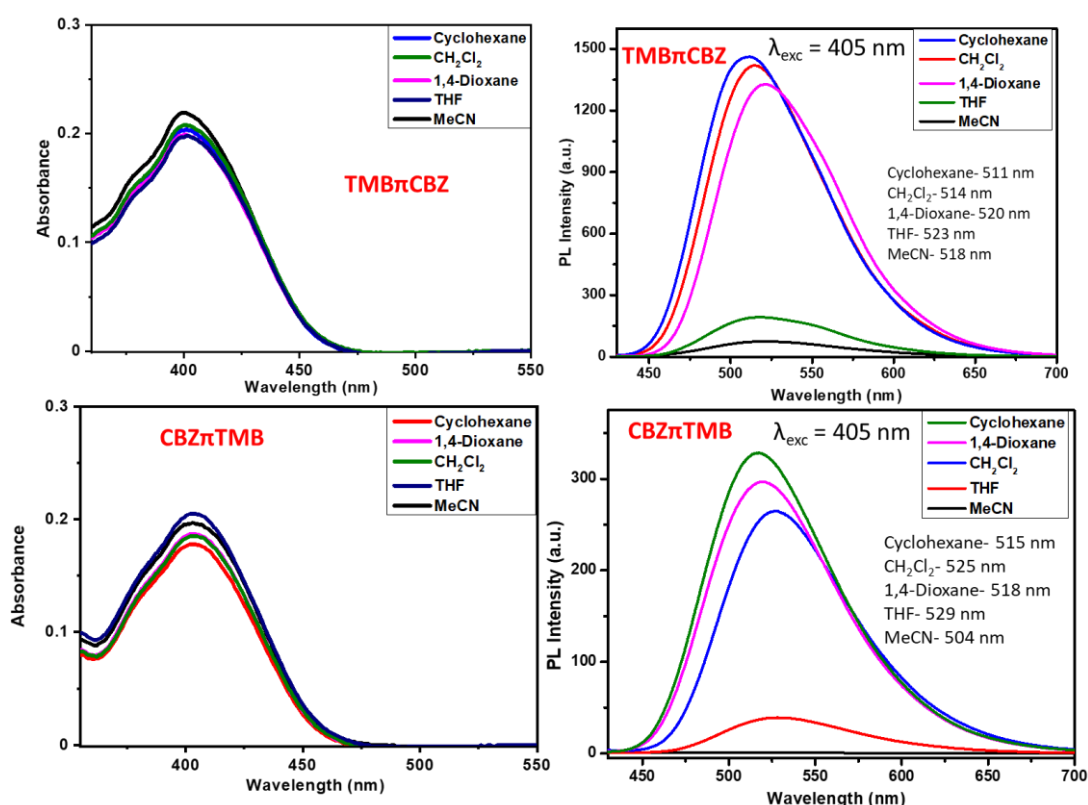


Fig S2: Absorbance and emission spectra of both the positional isomers in different polar solvents.

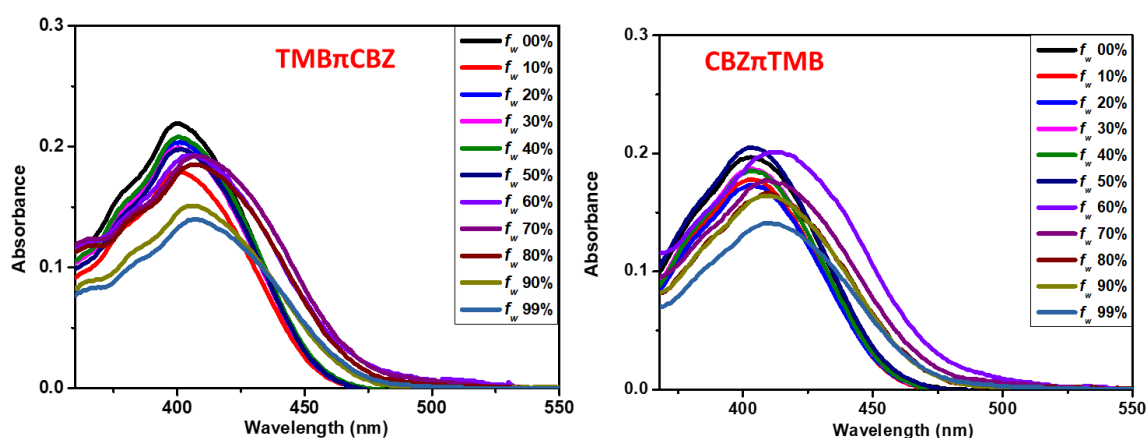


Fig S3: Absorption spectra of the compounds. 10 μ M acetonitrile solution upon gradual addition of water fraction [a nonsolvent f_w (v/v%)]

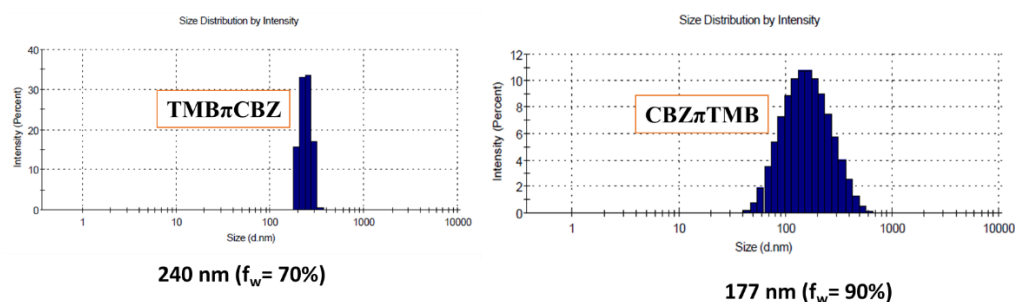


Fig S4: DLS studies for TMB π CBZ and CBZ π TMB at $f_w = 70\%$ and $f_w = 90\%$ respectively.

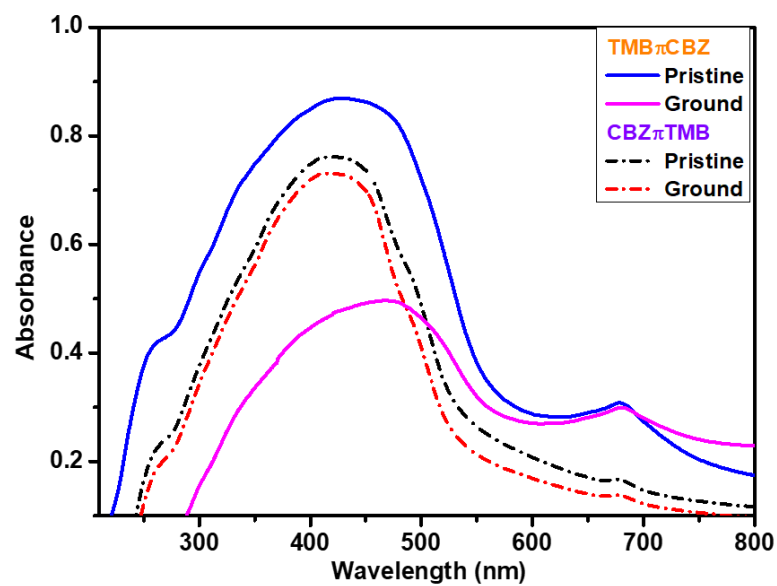


Fig S5: solid-state absorption spectra for TMB π CBZ and CBZ π TMB before and after grinding

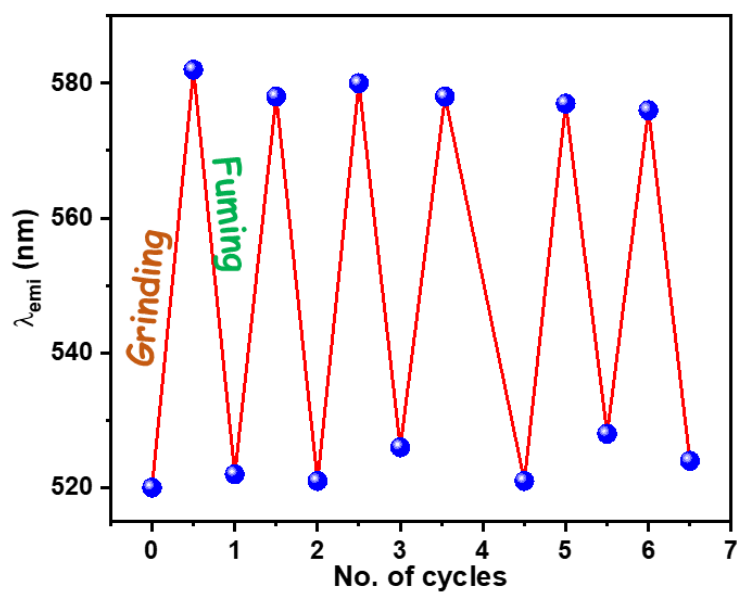


Fig S6: The plot of maximum emission wavelength changes with multiple grinding/Fuming process.

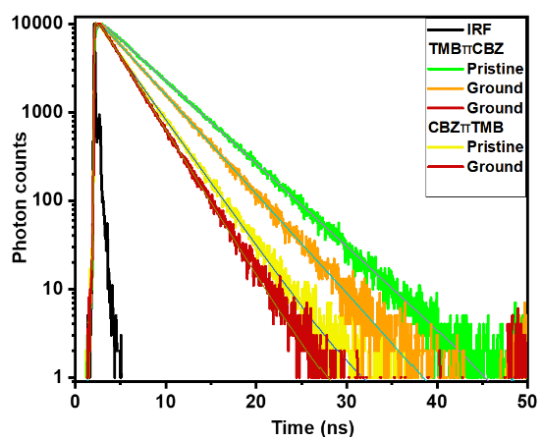


Fig S7: Solid-state lifetime decay for **TMB π CBZ** and **CBZ π TMB**

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 **TMB π CBZ** and **CBZ π TMB**

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
$V/\text{\AA}^3$	1626.71(8)	3176.69(10)
Z	2	4
$D_{\text{calc}}/\text{g cm}^{-3}$	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 [$I > 2\sigma(I)$]	0.0396	0.0501
wR2 [all data]	0.1116	0.1438
Max./min. residual electron dens. [$\text{e}\text{\AA}^{-3}$]	0.327/-0.238	0.326/-0.263

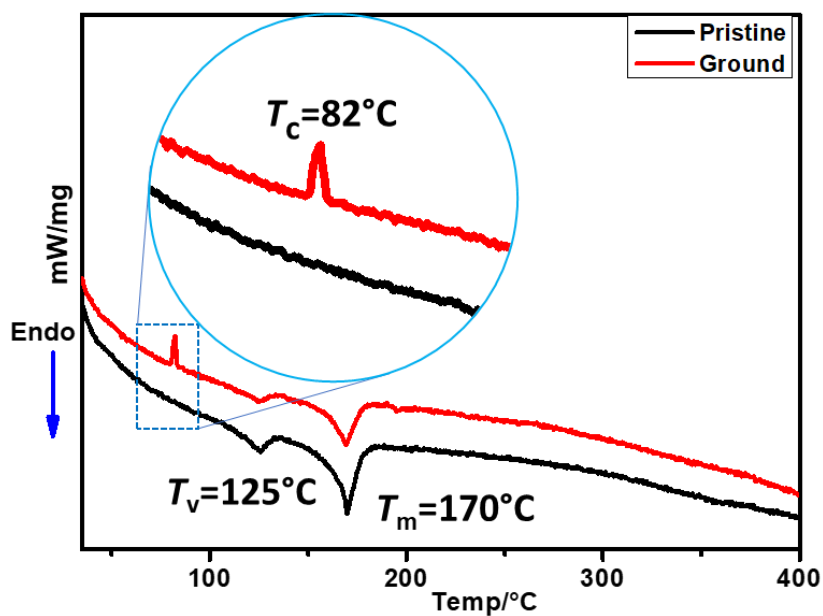


Fig S8: DSC thermogram for PFC-active TMB π CBZ in pristine and ground state.

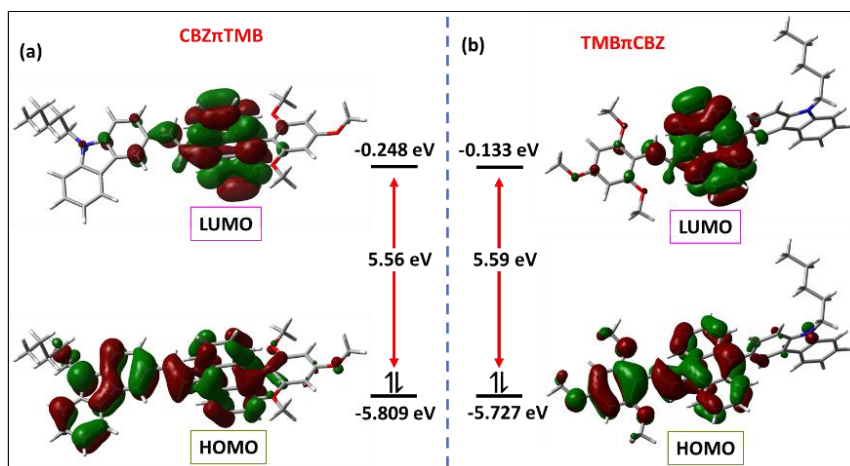


Fig S9: Molecular Orbital diagram for **TMBπCBZ** and **CBZπTMB**

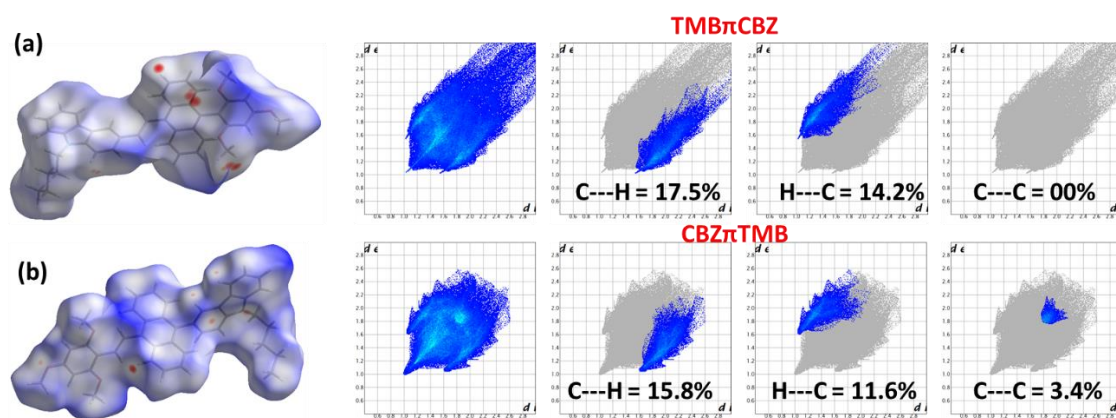


Fig S10: (a) d_{norm} Hirshfeld surface for **TMBπCBZ** and their 2D finger plots of C...H, H...C and C...C interactions, (b) d_{norm} Hirshfeld surface for **CBZπTMB** and their 2D finger plots of C...H, H...C and C...C interactions

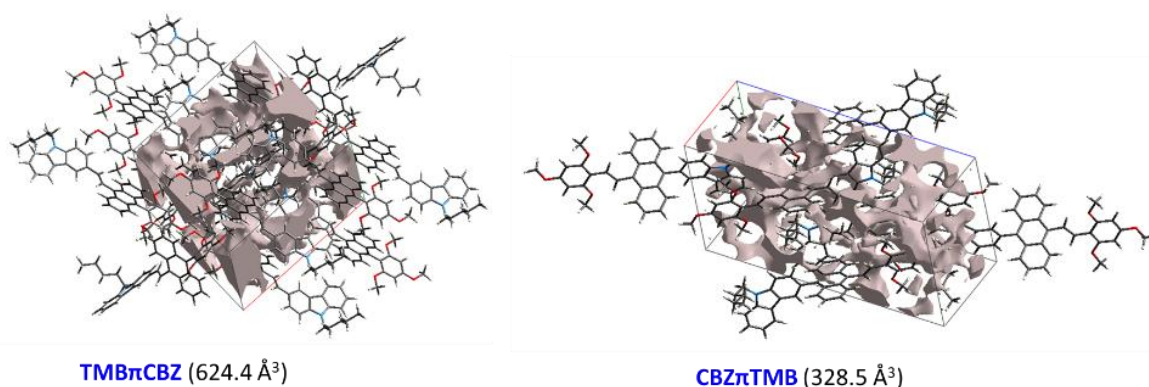


Fig S11: Void space for the isomers calculated from crystal Explorer 17.

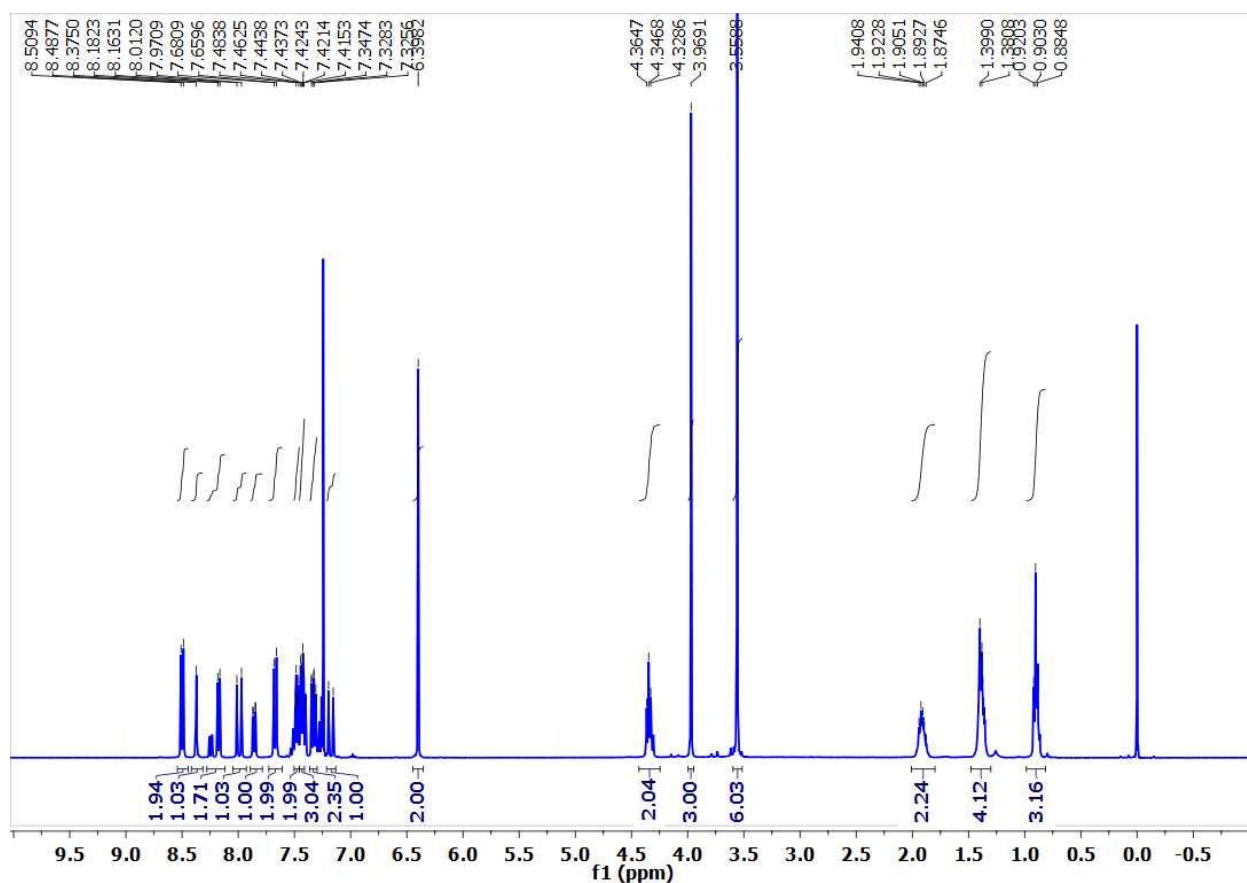


Fig S12: ¹H NMR spectrum for **TMBπCBZ** in CDCl₃

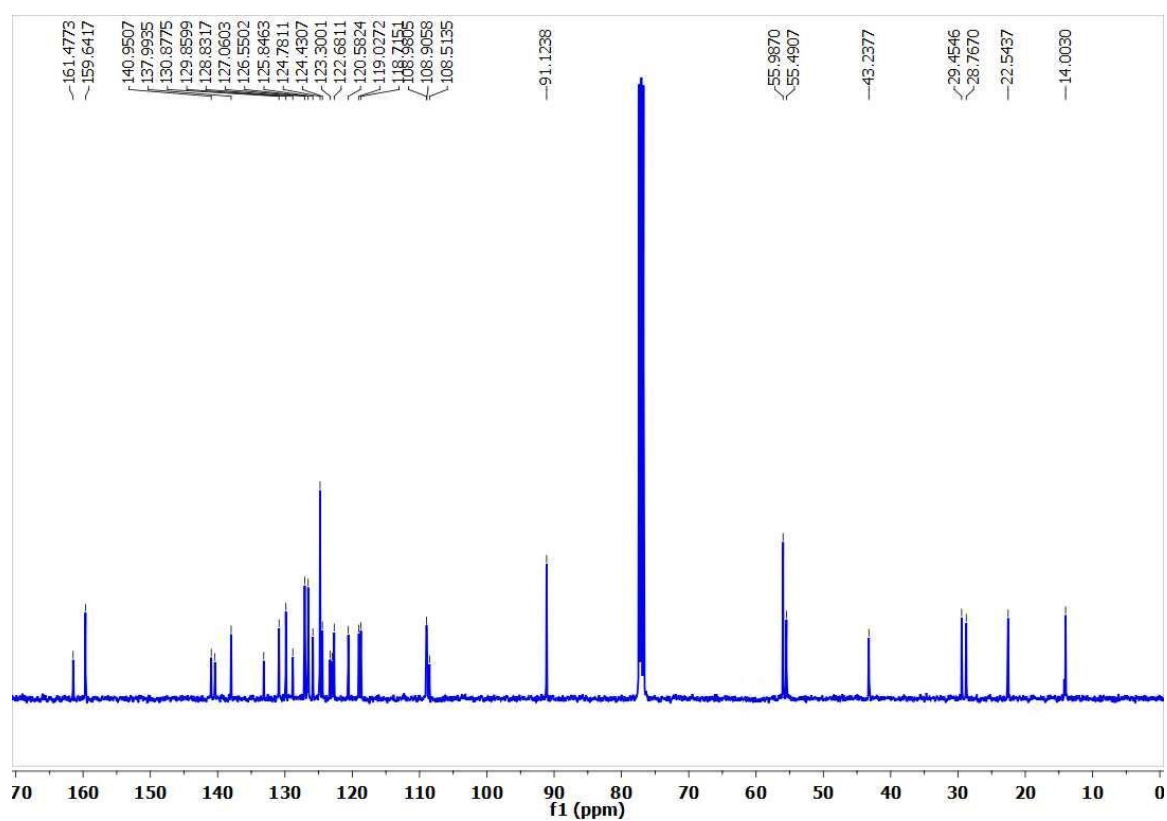


Fig S13: ¹³C NMR spectrum for **TMBπCBZ** in CDCl₃

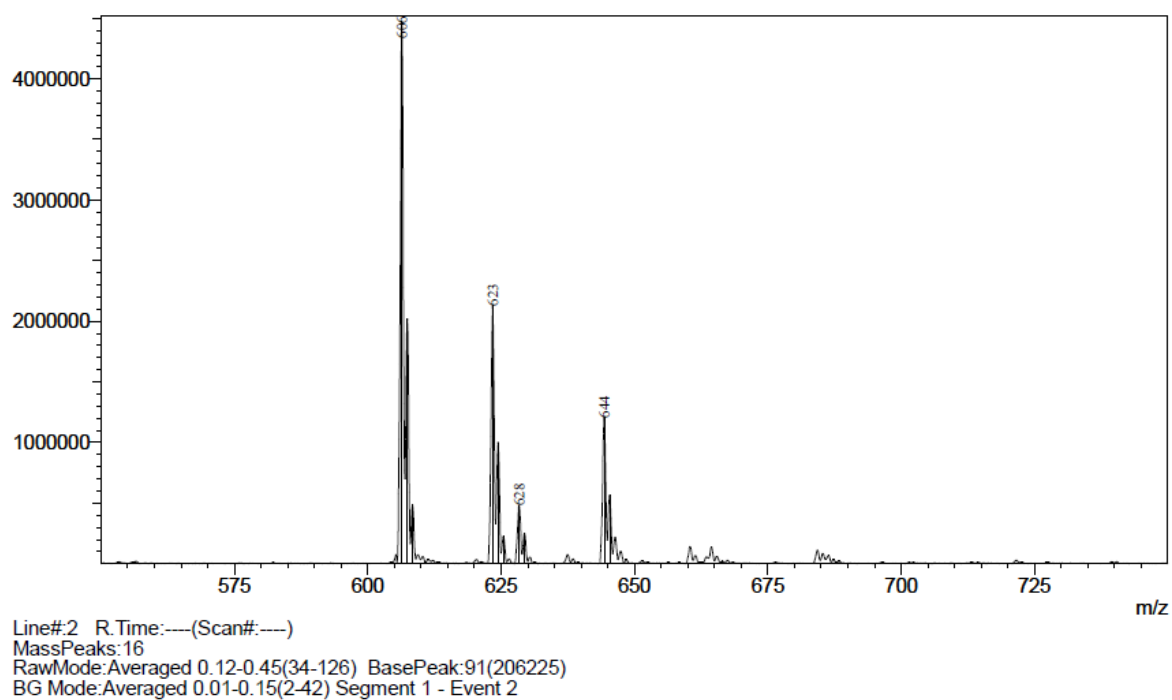


Fig S14: ESI-MS spectrum for **TMB π CBZ**

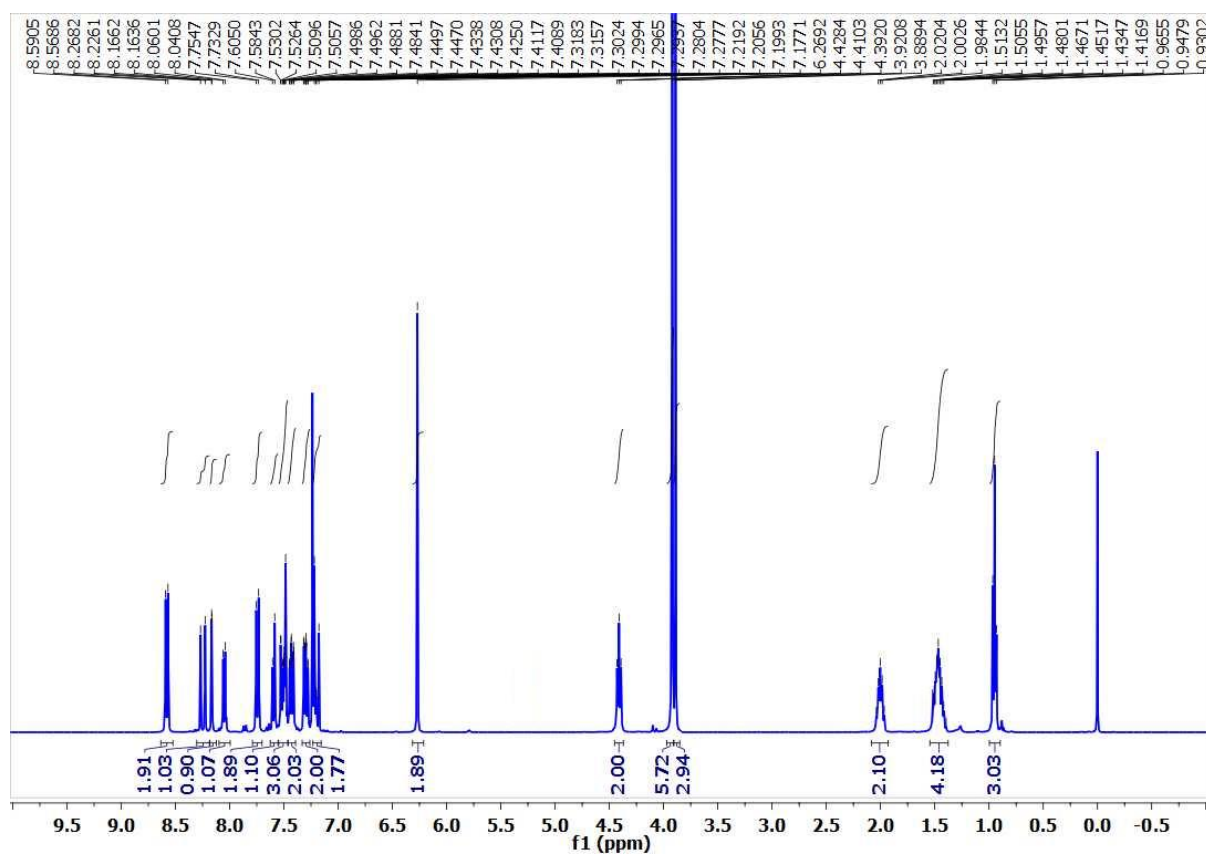


Fig S15: ^1H NMR spectrum for **CBZ π TMB** in CDCl_3

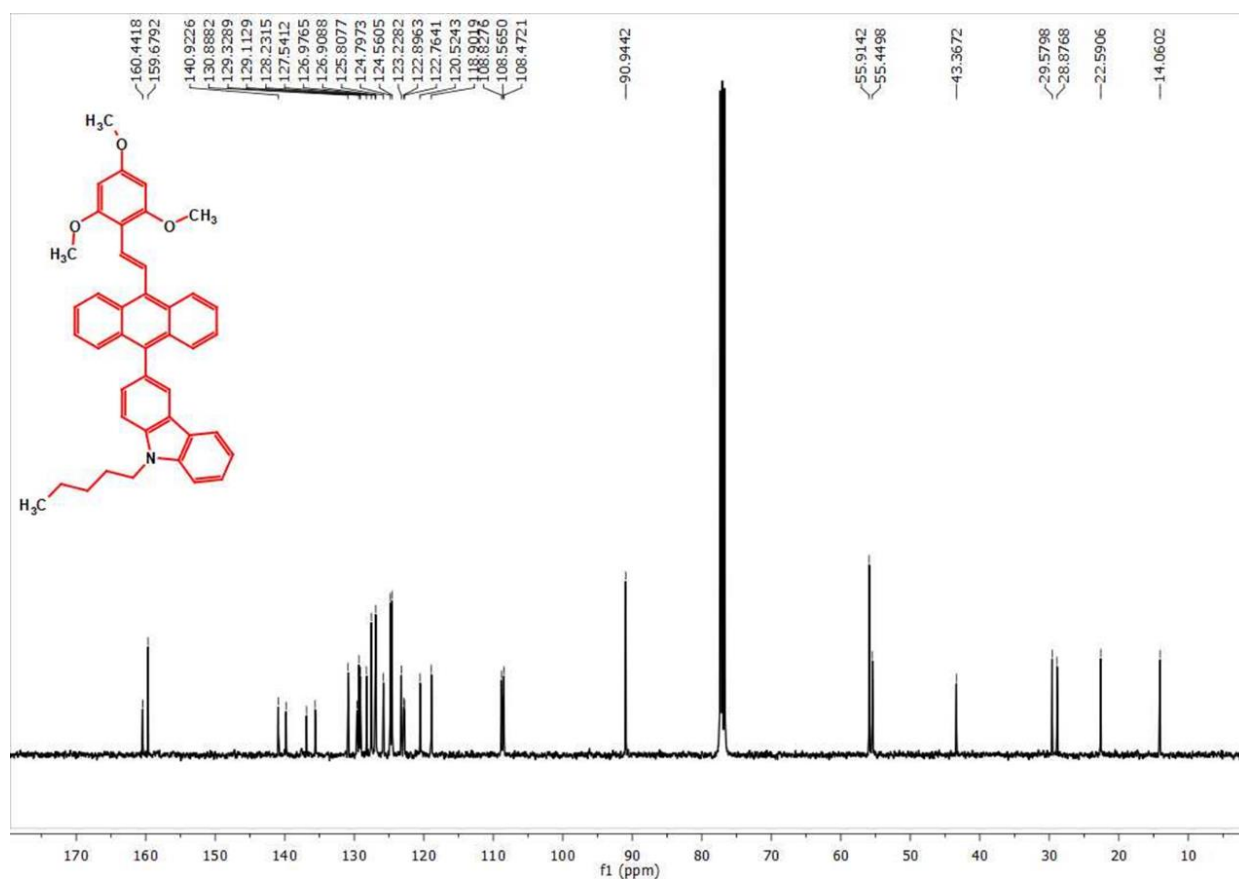


Fig S16: ^{13}C NMR spectrum for **CBZ π TMB** in CDCl_3

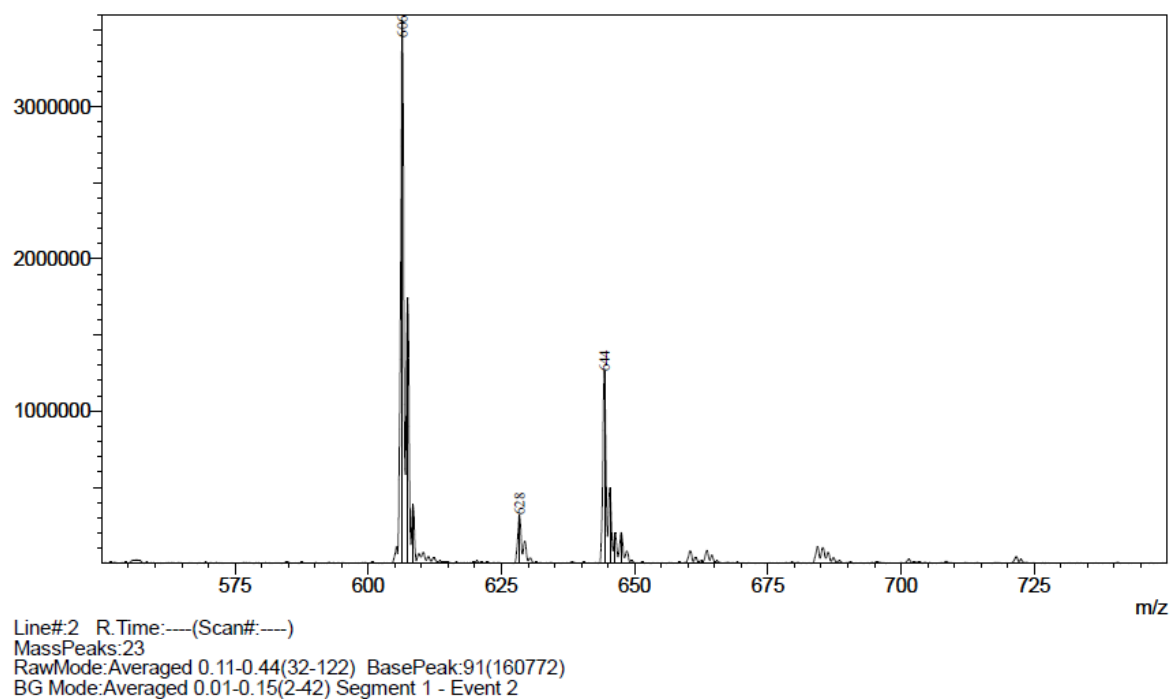


Fig S17: ESI-MS spectrum for **CBZ π TMB**

END