

## Novel Hole Transporting Materials Based on Triptycene Core for High Efficiency Mesoscopic Perovskite Solar Cells

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### Supporting Information

**Figure S1.**  $^1\text{H}$  NMR spectrum of 2,6,14-Tri(thien-2-yl)-triptycene.

**Figure S2.**  $^{13}\text{C}$  NMR spectrum of 2,6,14-Tri(thien-2-yl)-triptycene.

**Figure S3.**  $^1\text{H}$  NMR spectrum of T101.

**Figure S4.**  $^{13}\text{C}$  NMR spectrum of T101.

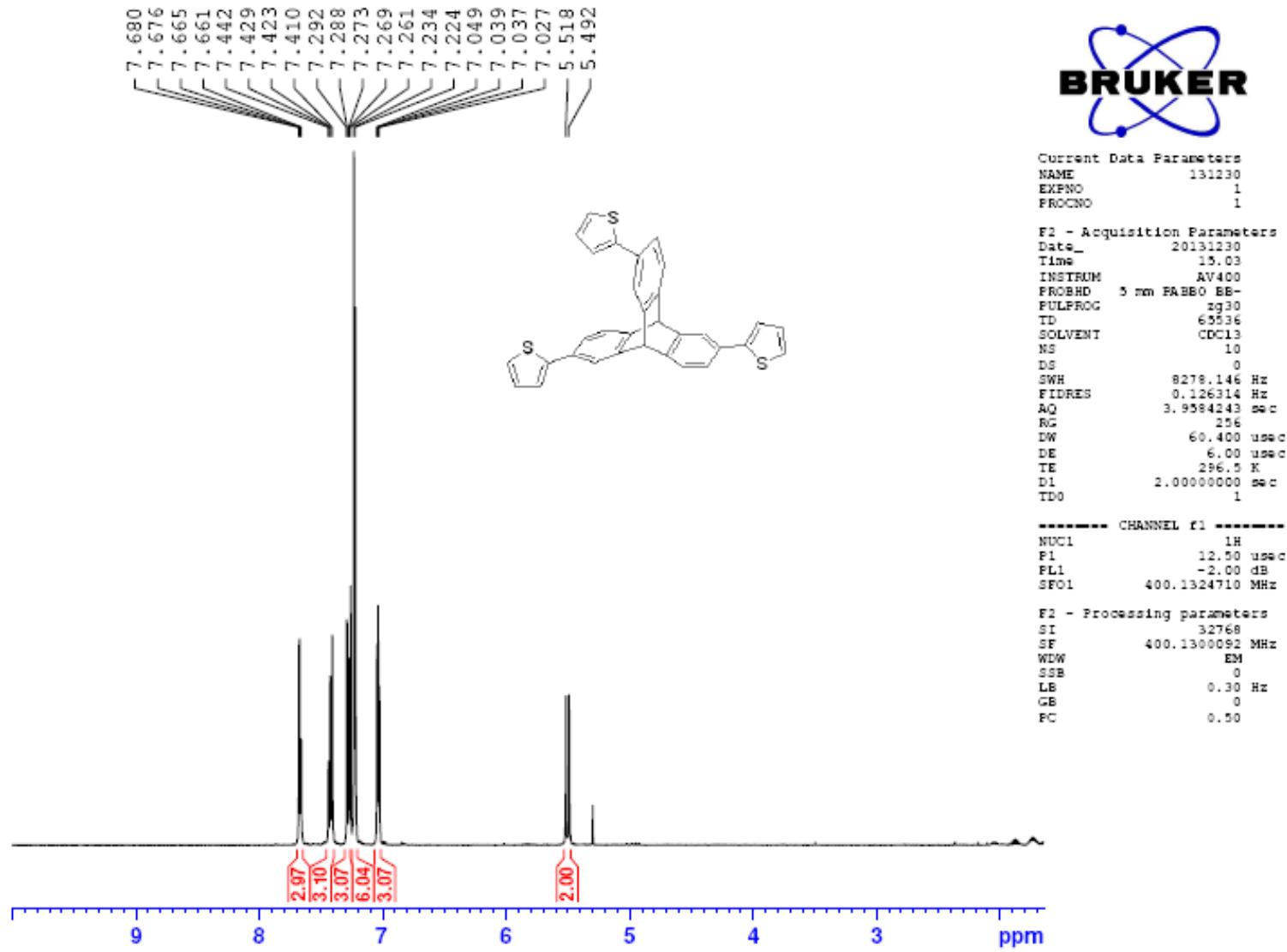
**Figure S5.**  $^1\text{H}$  NMR spectrum of T102.

**Figure S6.**  $^{13}\text{C}$  NMR spectrum of T102.

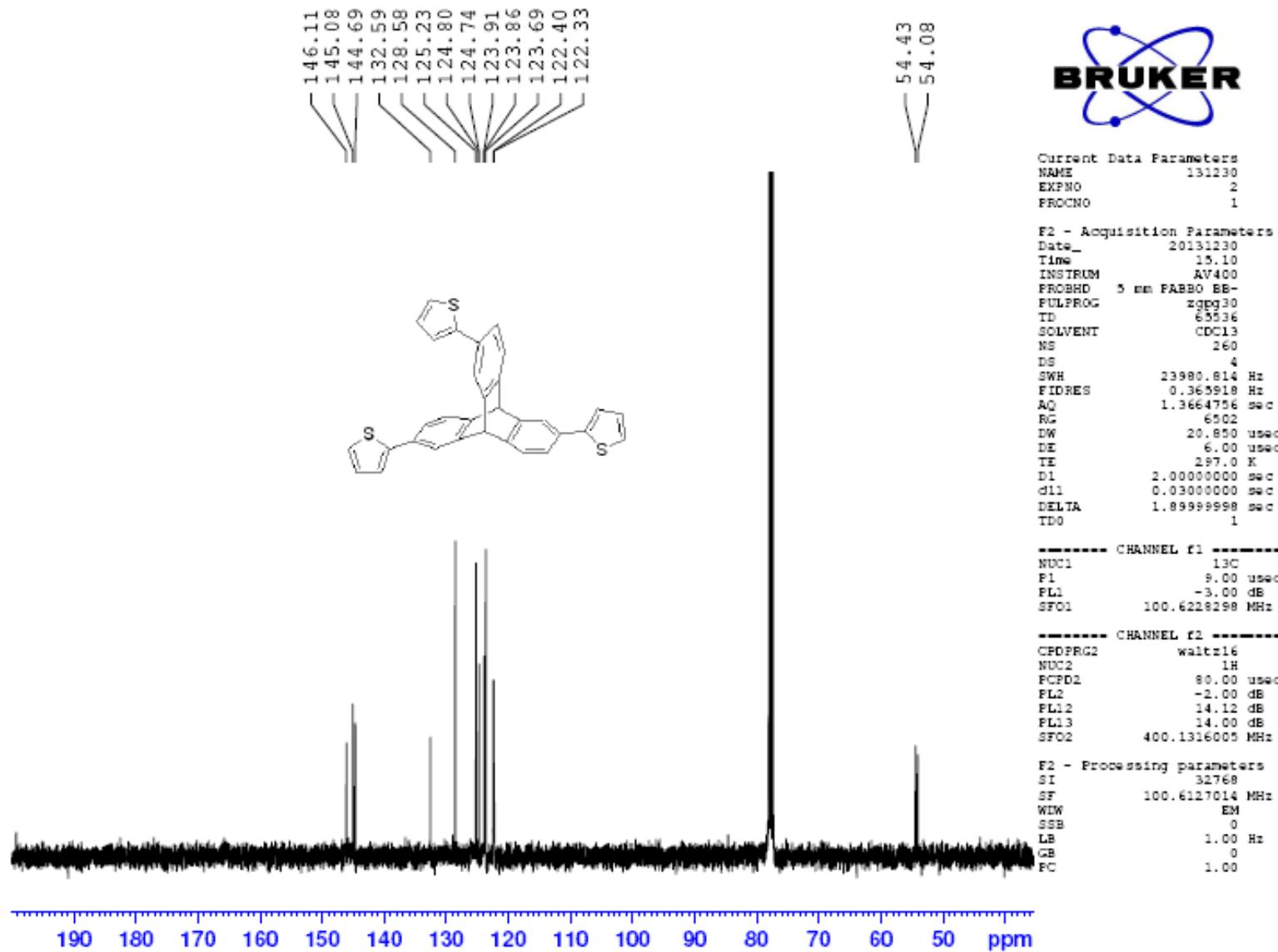
**Figure S7.**  $^1\text{H}$  NMR spectrum of T103.

**Figure S8.**  $^{13}\text{C}$  NMR spectrum of T103.

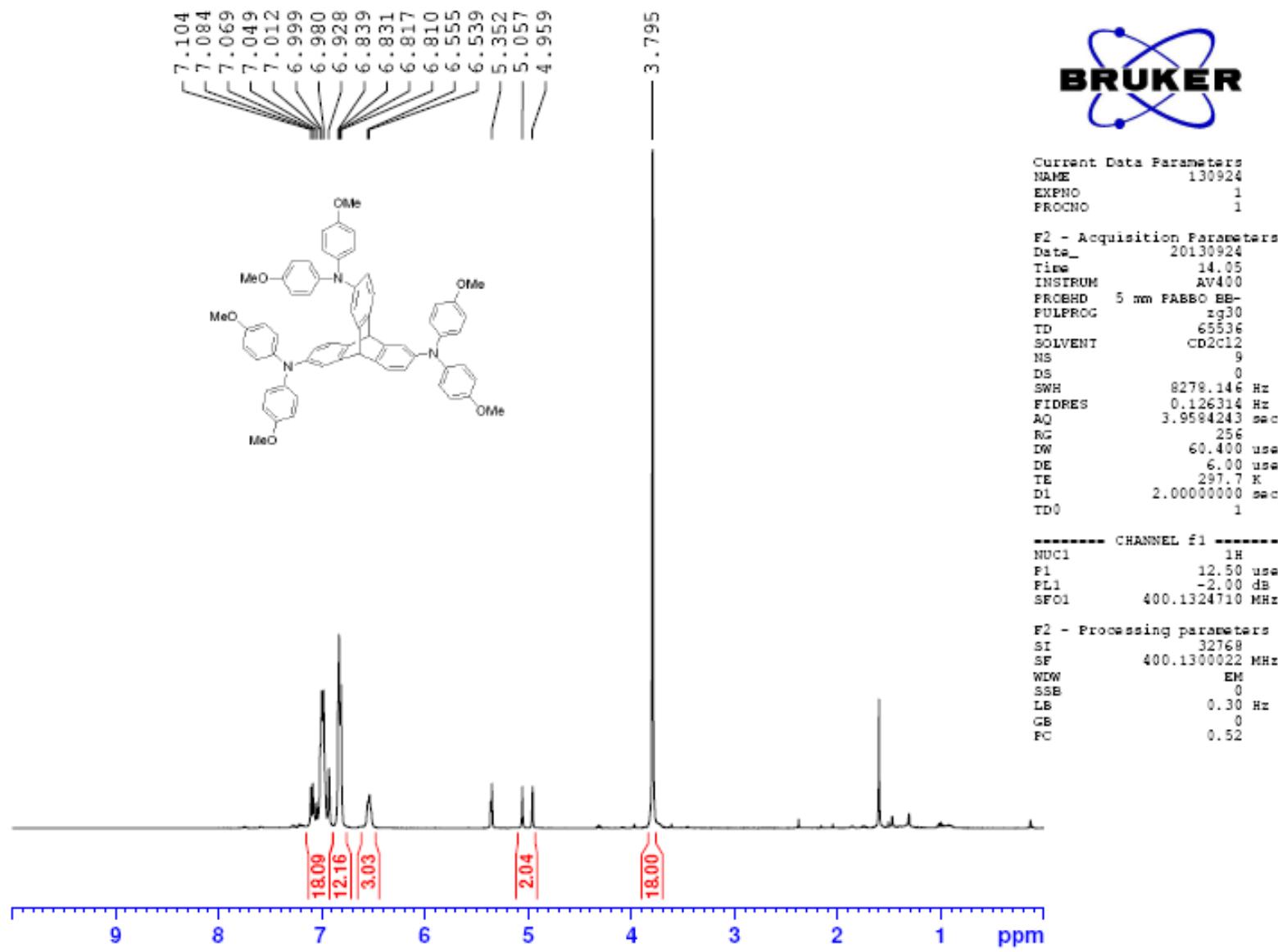
**Figure S9.** Natural Transition Orbitals (NTOs) for the dominant transitions of triptycene-based materials at CAM-B3LYP/6-31G(d,p) level of theory.



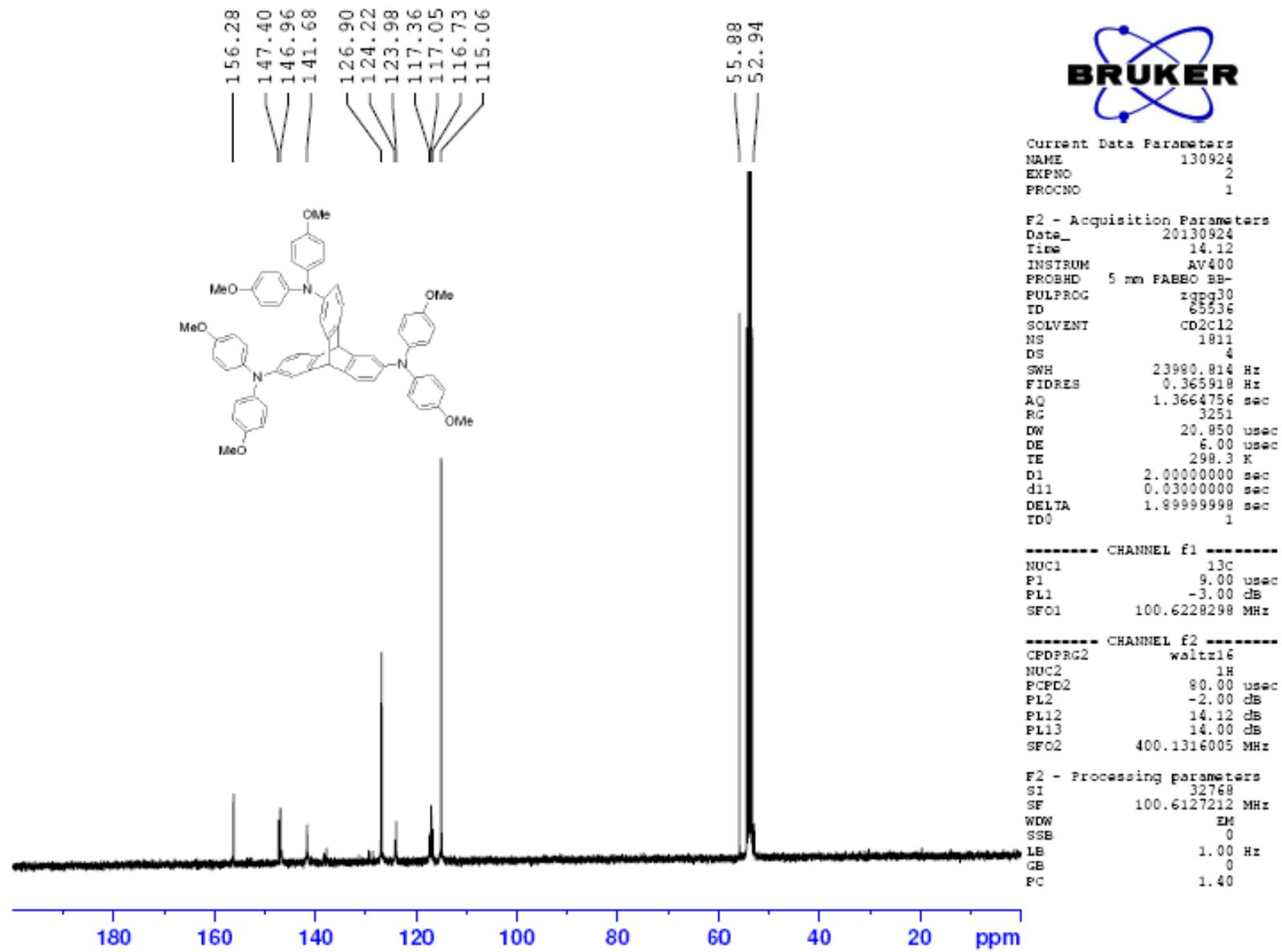
**Figure S1.**  $^1\text{H}$  NMR spectrum of 2,6,14-Tri(thien-2-yl)-triptycene.



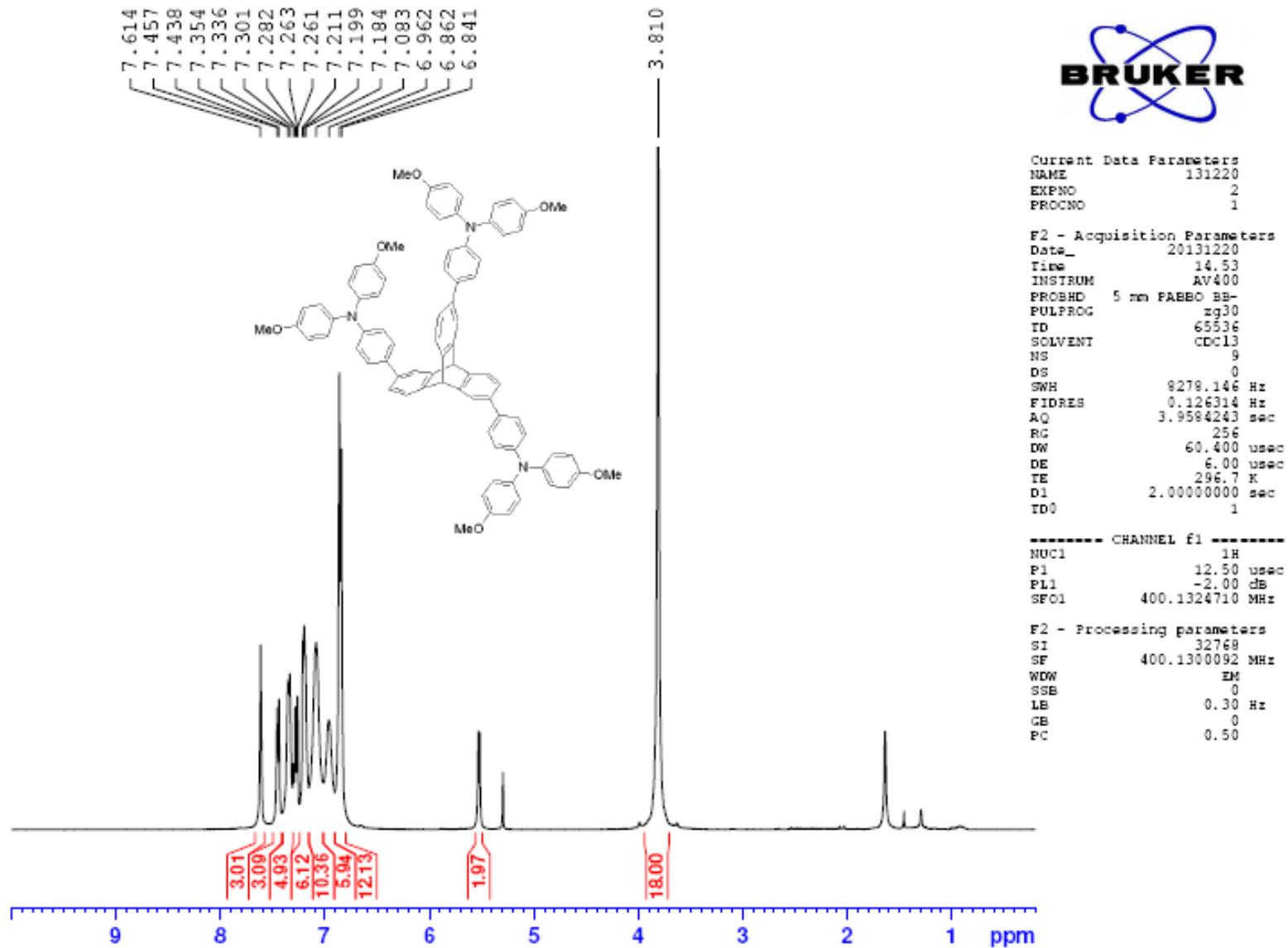
**Figure S2.**  $^{13}\text{C}$  NMR spectrum of 2,6,14-Tri(thien-2-yl)-triptycene.



**Figure S3.**  $^1\text{H}$  NMR spectrum of T101.



**Figure S4.**  $^{13}\text{C}$  NMR spectrum of T101.



**Figure S5.**  $^1\text{H}$  NMR spectrum of T102.

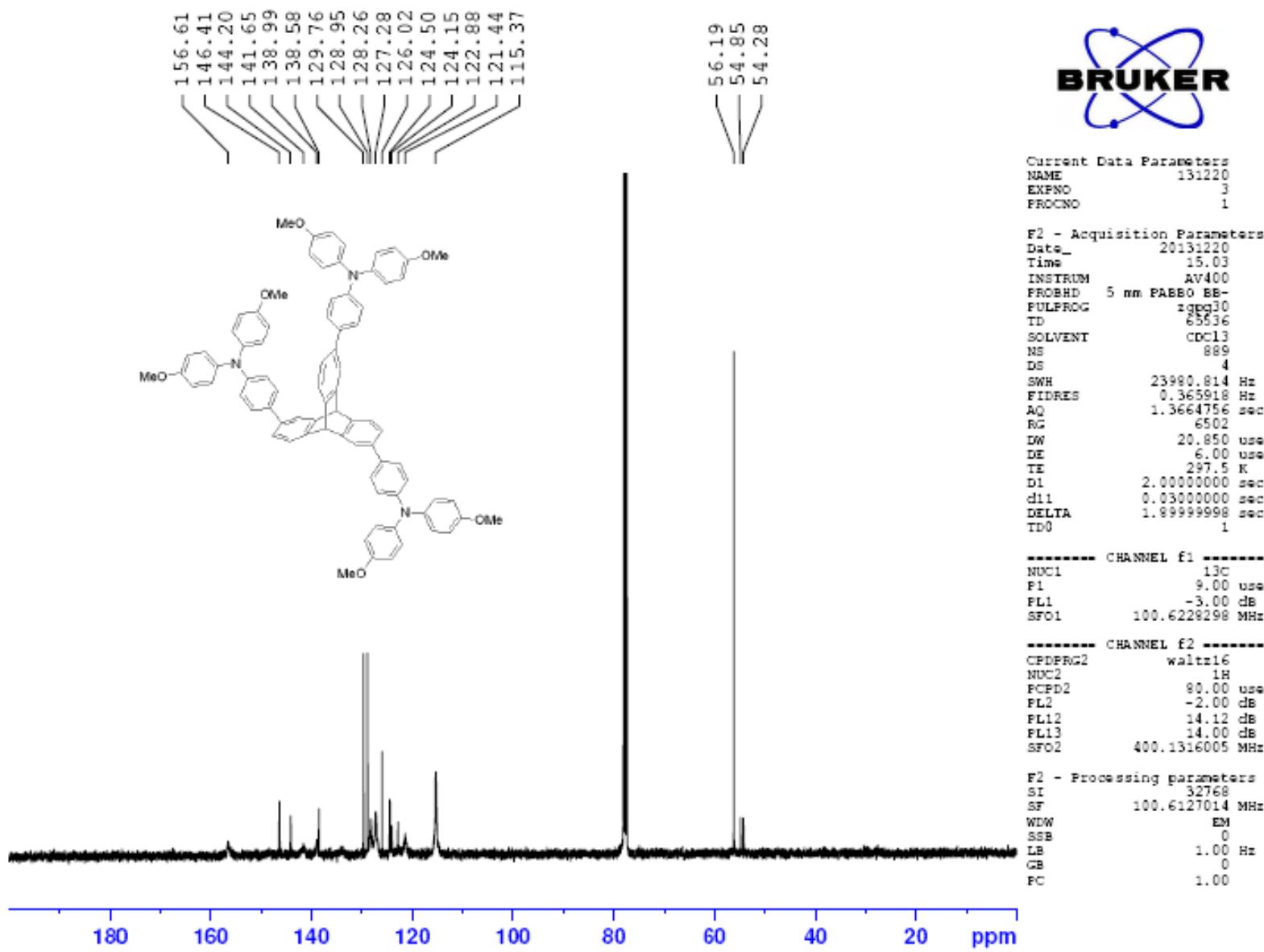


Figure S6.  $^{13}\text{C}$  NMR spectrum of T102.

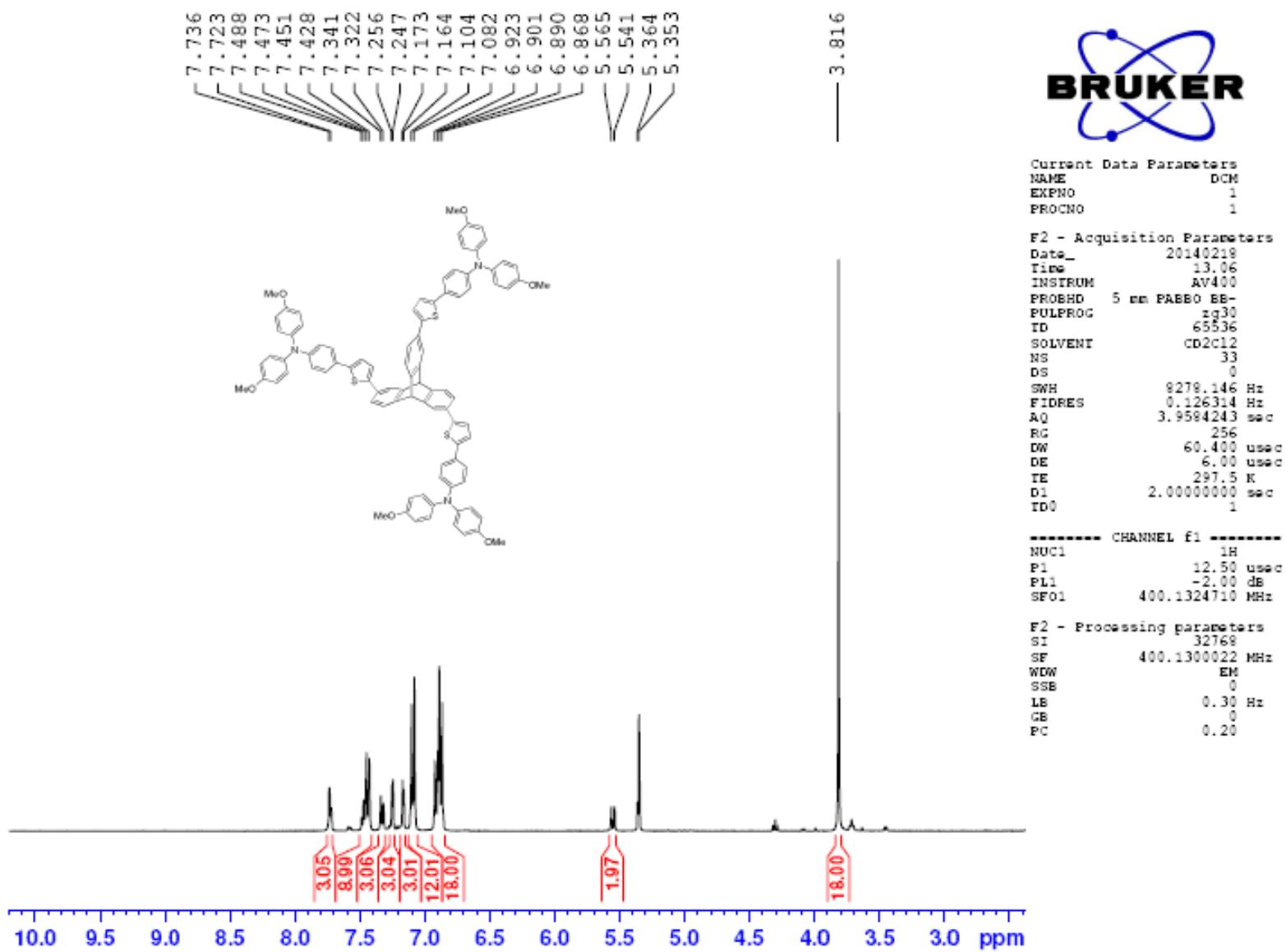


Figure S7.  $^1\text{H}$  NMR spectrum of T103.

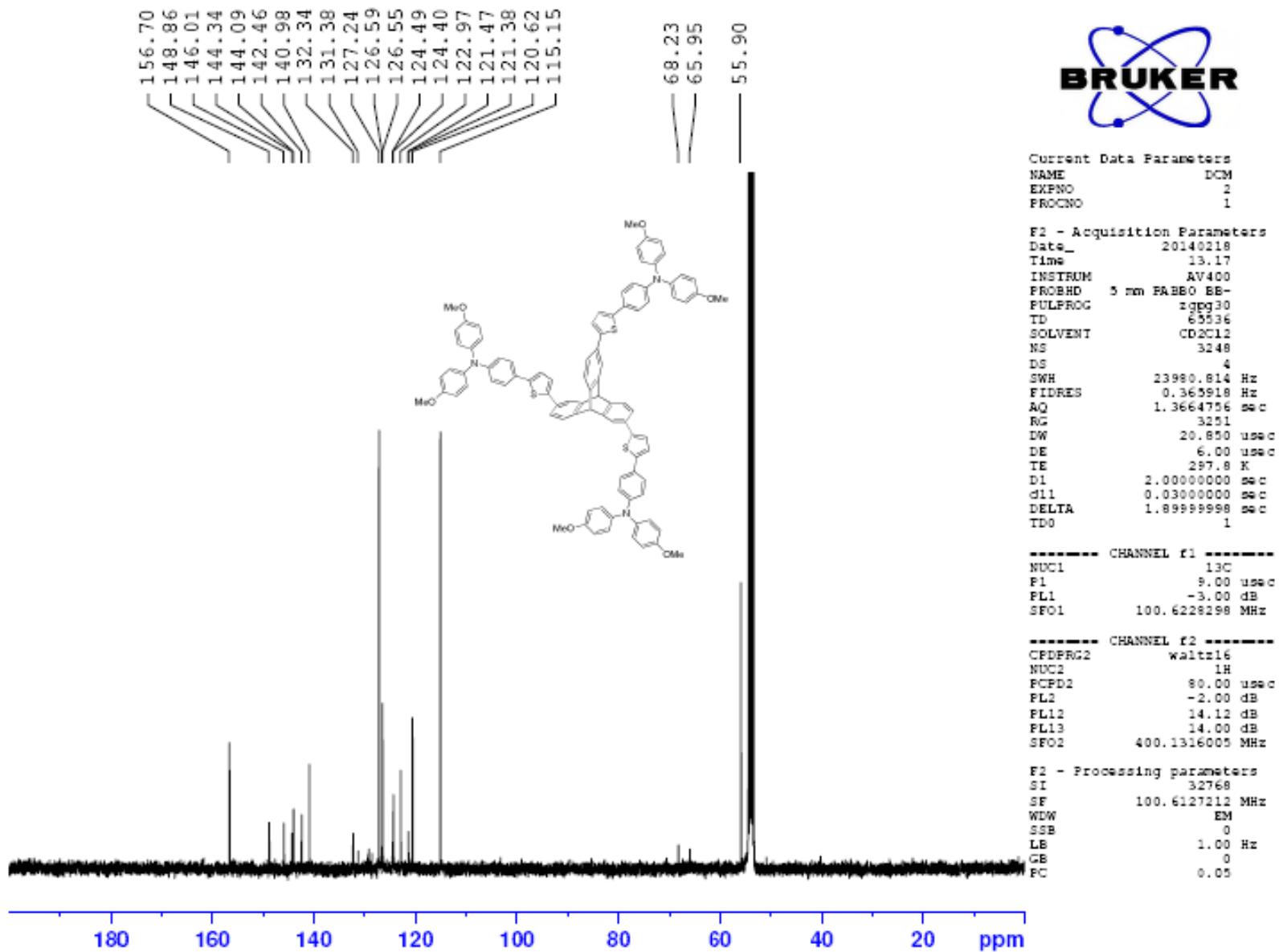
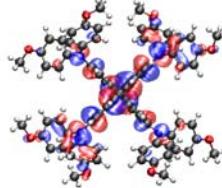
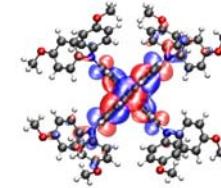
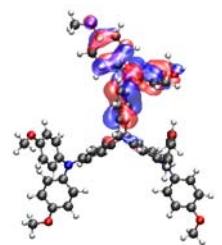
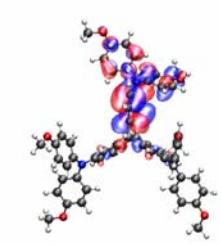
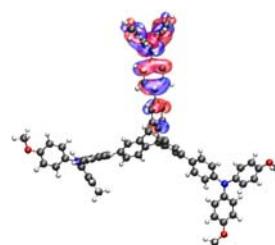
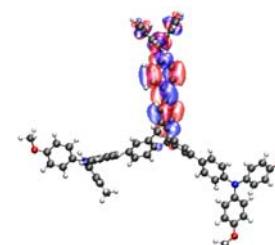
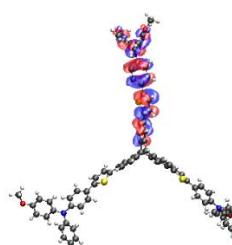
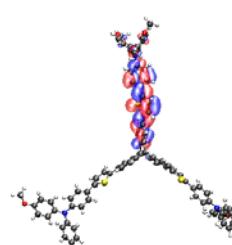


Figure S8.  $^{13}\text{C}$  NMR spectrum of T103.

Molecule	$\Delta E(\text{eV})$	$f$	Hole	Particle
Spiro-OMeTAD	3.64	1.29		
T101	4.32	1.18		
T102	3.99	1.91		
T103	3.43	2.69		

**Figure S9.** Natural Transition Orbitals (NTOs) for the dominant transitions of triptycene-based materials at CAM-B3LYP/6-31G(d,p) level of theory.