

Supporting information for

**Photophysical and photovoltaic properties of truxene-functionalized  
conjugated polymer–fullerene supramolecules**

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## 1. $^{13}\text{C}$ NMR spectra of M1, M3 and M4

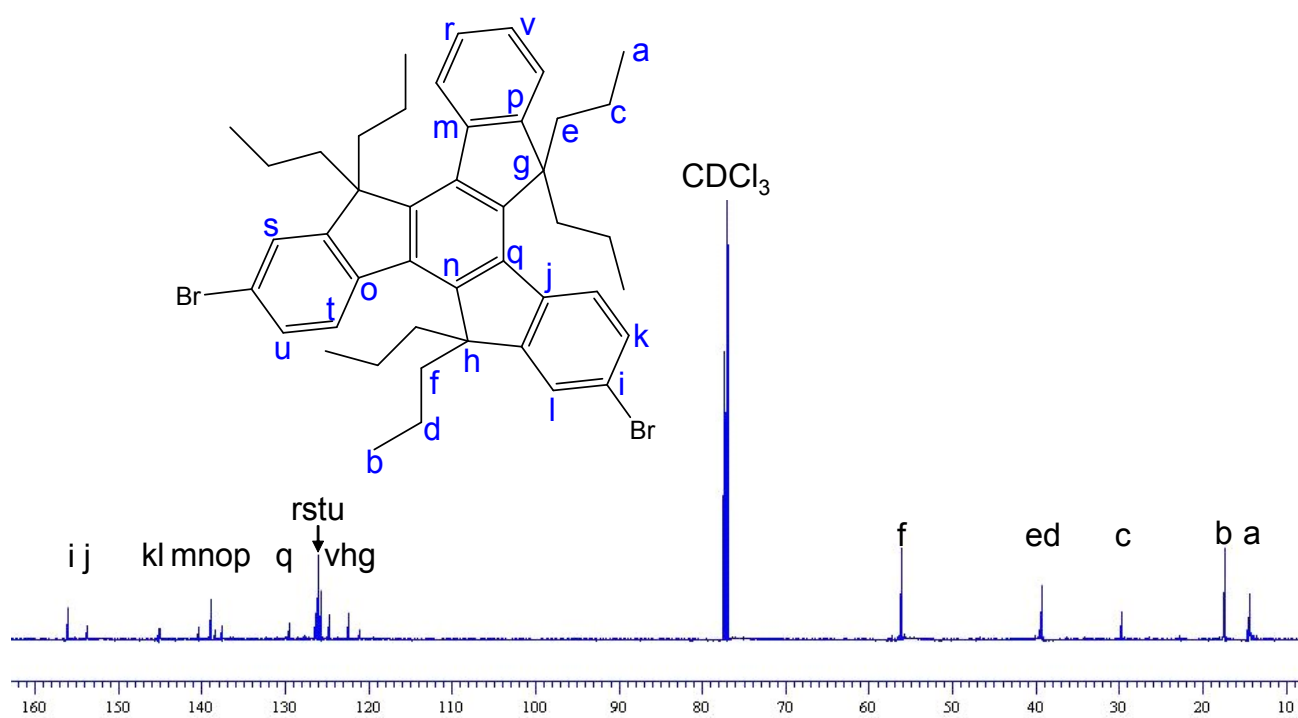


Fig. S1  $^{13}\text{C}$  NMR spectrum of M1.

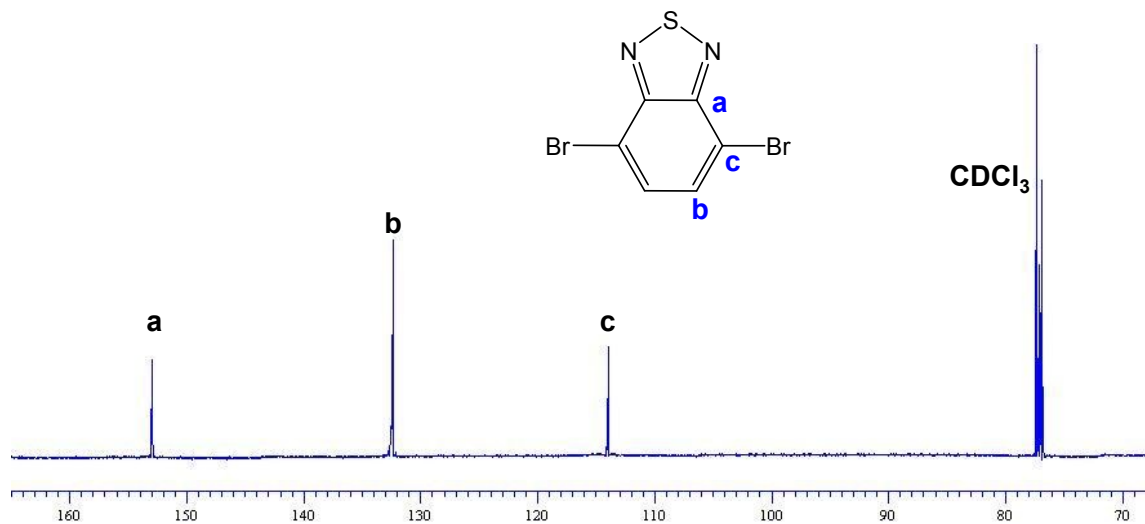
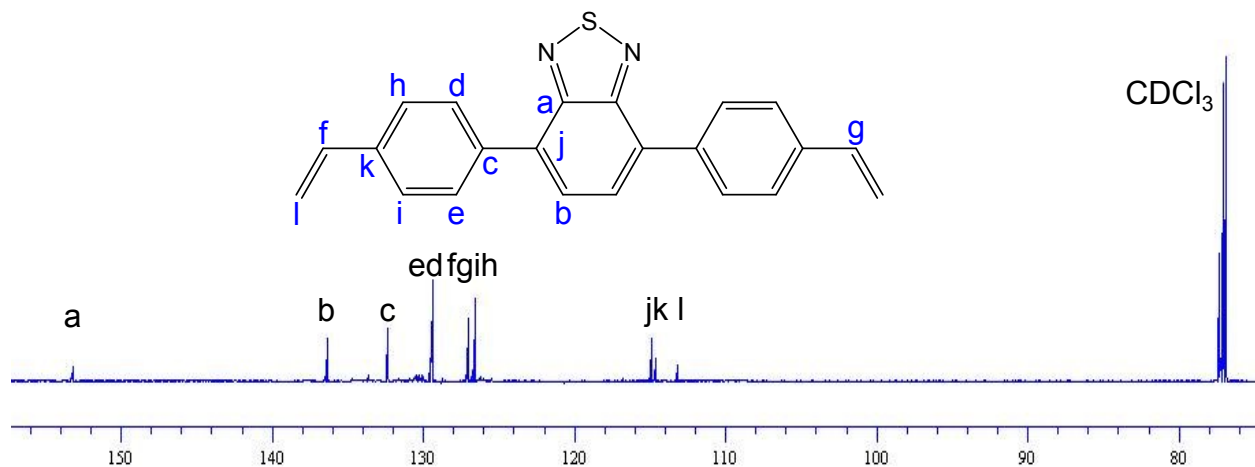
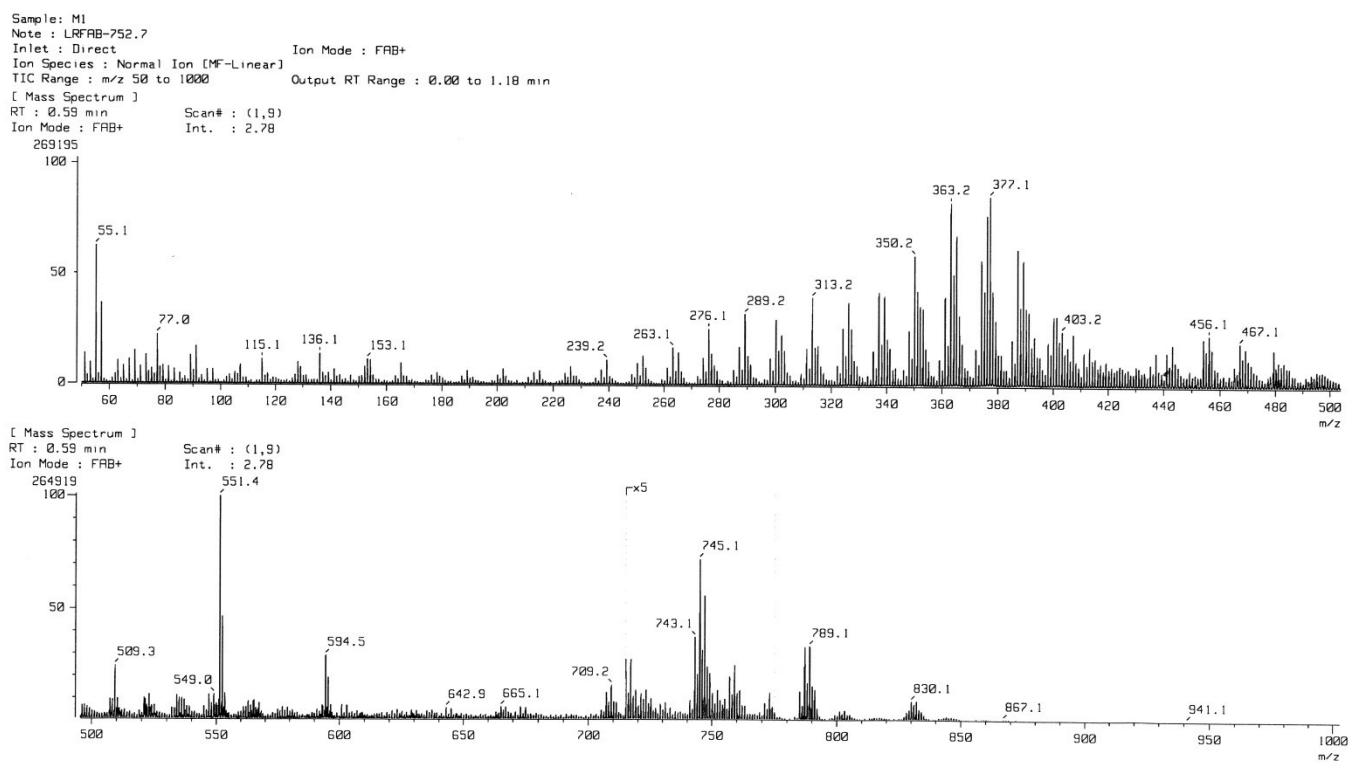


Fig. S2  $^{13}\text{C}$  NMR spectrum of M3.



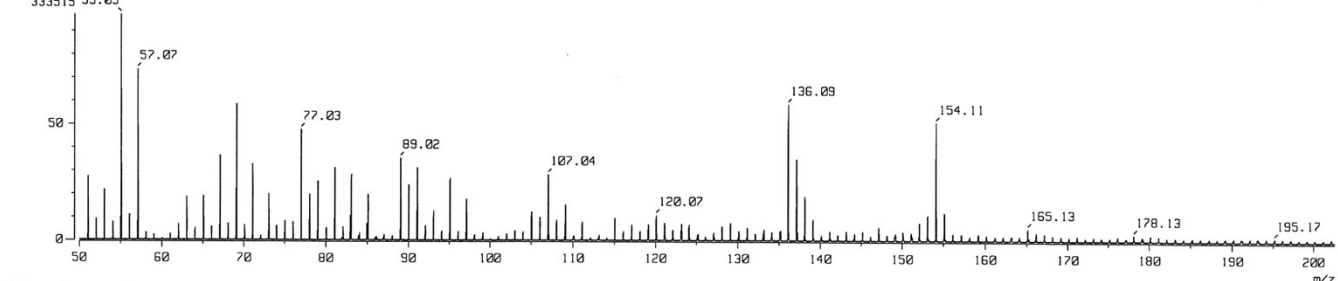
**Fig. S3** <sup>13</sup>C NMR spectrum of M4.

## 2. FABMS spectra of M1, M3 and M4



**Fig. S4** FABMS spectrum of M1.

Sample: M3  
 Note: LRFAB-293.9  
 Inlet: Direct Ion Mode: FAB+  
 Ion Species: Normal Ion [MF-Linear]  
 TIC Range: m/z 50 to 600 Output RT Range: 0.00 to 1.01 min  
 [ Mass Spectrum ]  
 RT: 0.51 min Scan#: (1,10)  
 Ion Mode: FAB+ Int.: 3.28



[ Mass Spectrum ]  
 RT: 0.51 min Scan#: (1,10)  
 Ion Mode: FAB+ Int.: 3.28

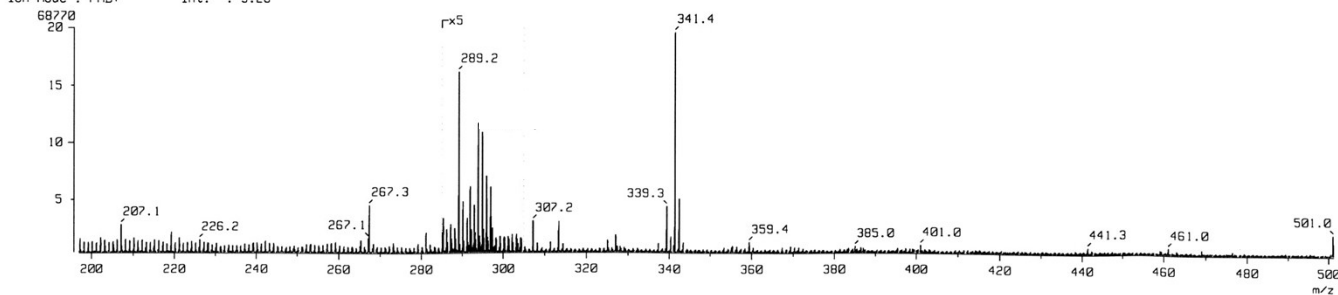
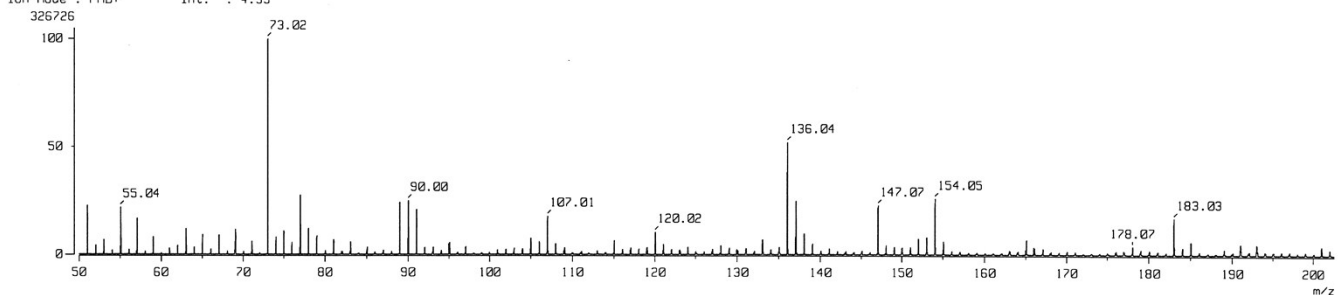


Fig. S5 FABMS spectrum of M3.

Sample: M4  
 Note: LRFAB-340.1  
 Inlet: Direct Ion Mode: FAB+  
 Ion Species: Normal Ion [MF-Linear]  
 TIC Range: m/z 50 to 600 Output RT Range: 0.00 to 0.56 min  
 [ Mass Spectrum ]  
 RT: 0.28 min Scan#: (1,6)  
 Ion Mode: FAB+ Int.: 4.95



[ Mass Spectrum ]  
 RT: 0.28 min Scan#: (1,6)  
 Ion Mode: FAB+ Int.: 4.95

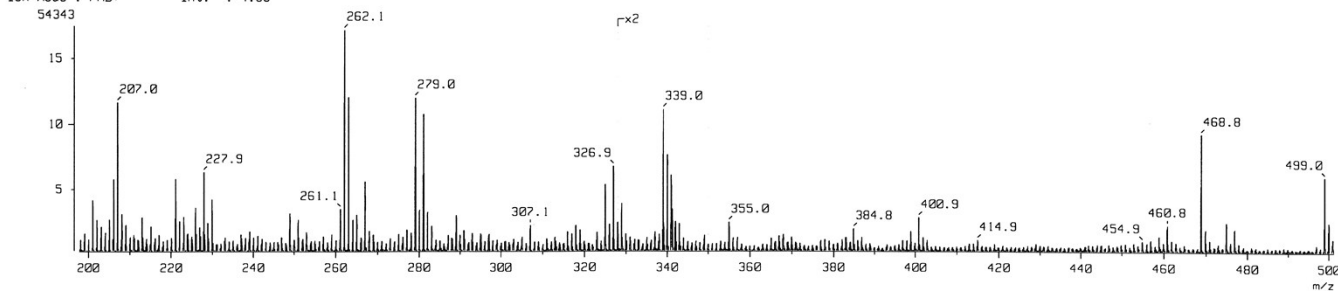
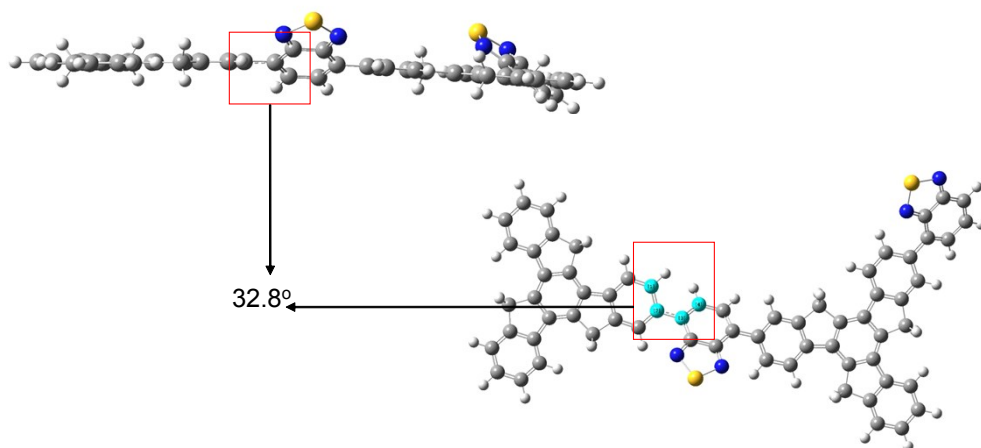
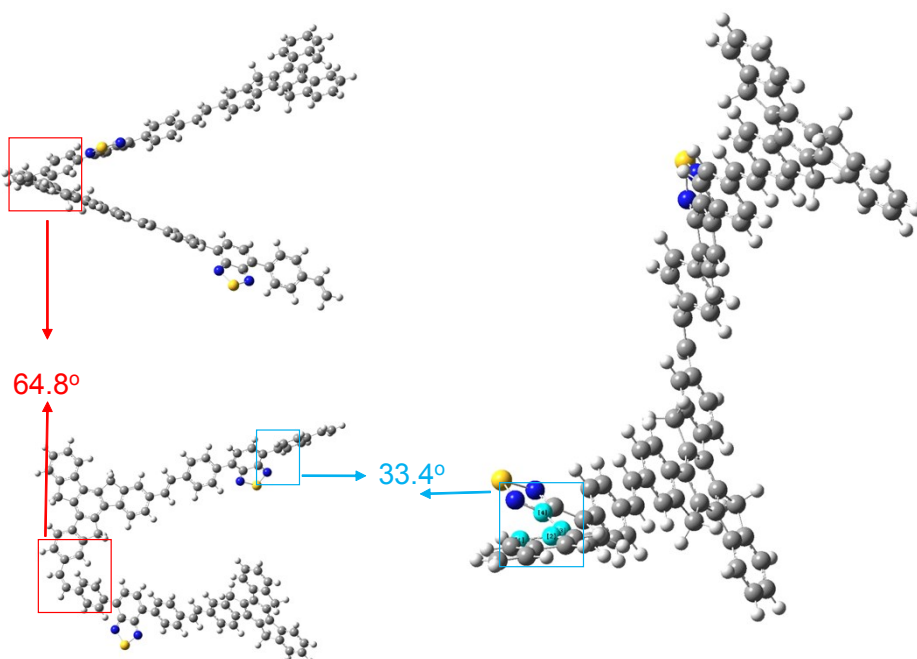


Fig. S6 FABMS spectrum of M4.

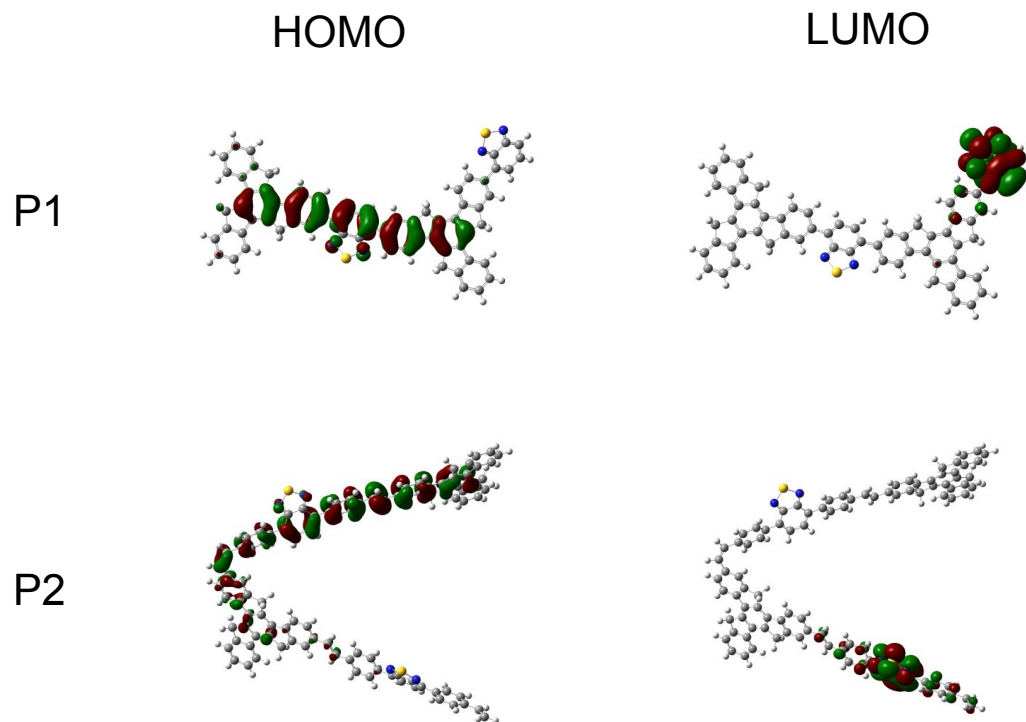
### 3. Typical optimized structure, HOMO, and LUMO



**Fig. S7** The optimized structure of D-A dimer in P1; the number is the dihedral angle in rectangular.



**Fig. S8** The optimized structure of D-A dimer in P2; the number is the dihedral angle in rectangular.



**Fig. S9** HOMO and LUMO orbitals for P1 and P2.