Supporting Information

Study on structure-performance relationship of nonlinear optical chromophore with different donors, bridges and acceptors

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Table of Contents

1. UV-Vis Absorption Spectroscopy

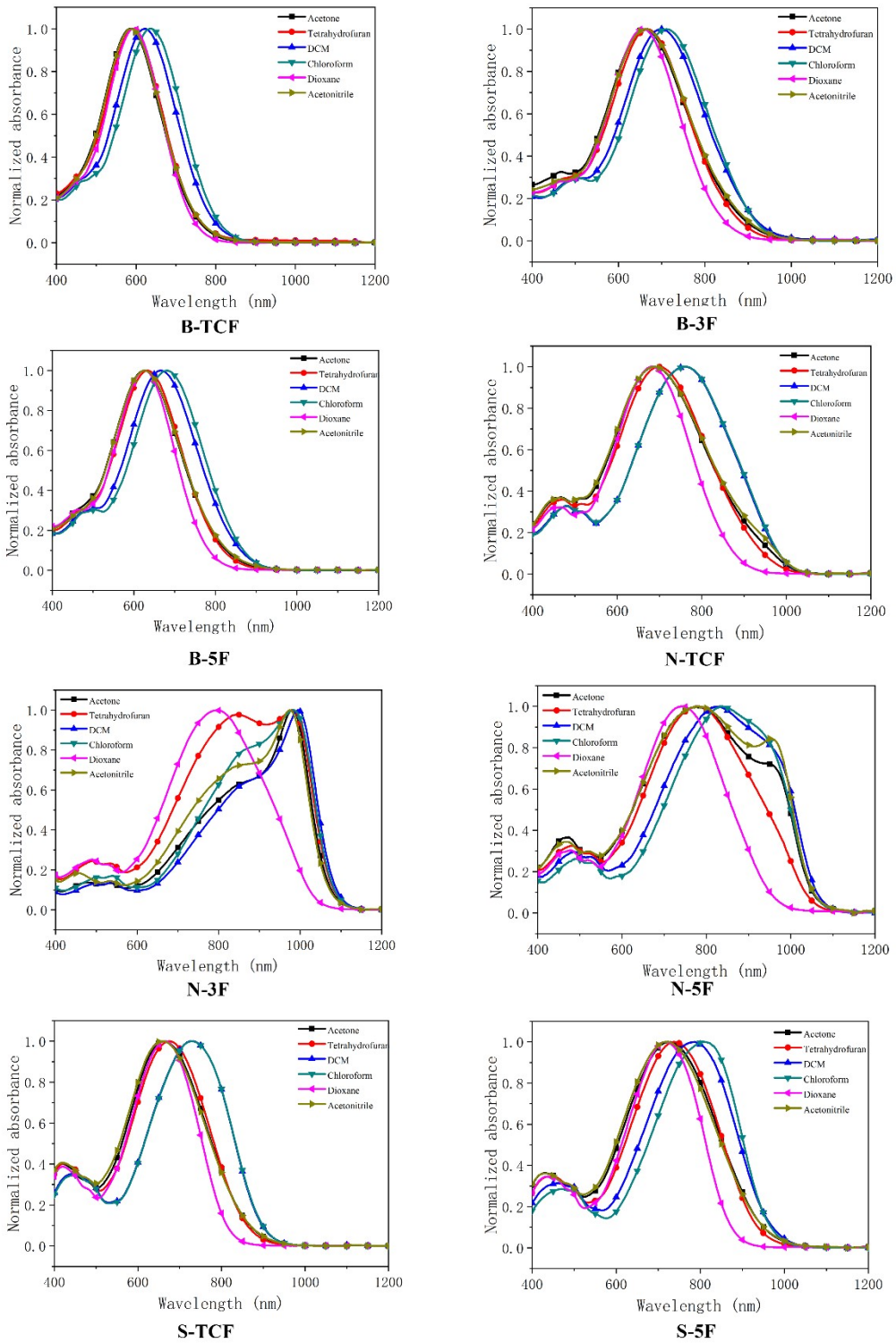

Figure S1. Normalized UV-Vis absorption spectra of the eight chromophores in six aprotic solvents with varying dielectric constants (ε)

2. DFT Calculations

Table S1 β value of chromophores in vacumm and solvents

Cmpd	Vac [a]	Thf [b]	Tol [c]	Chl [d]
B-TCF	888	3617	2347	3186
B-3F	1016	2553	1712	2274
B-5F	996	2310	1538	1942
N-TCF	1214	4648	2835	4003
N-3F	1405	4161	2639	3636
N-5F	1342	2993	1982	2655
S-TCF	905	4131	2355	3483
S-3F	1047	3279	2066	2857
S-5F	1042	2470	1748	2238

[abcd] was the first-order hyperpolarizability in vacuum、tetrahydrofuran、 chloroform and toluene calculated from DFT calculations.

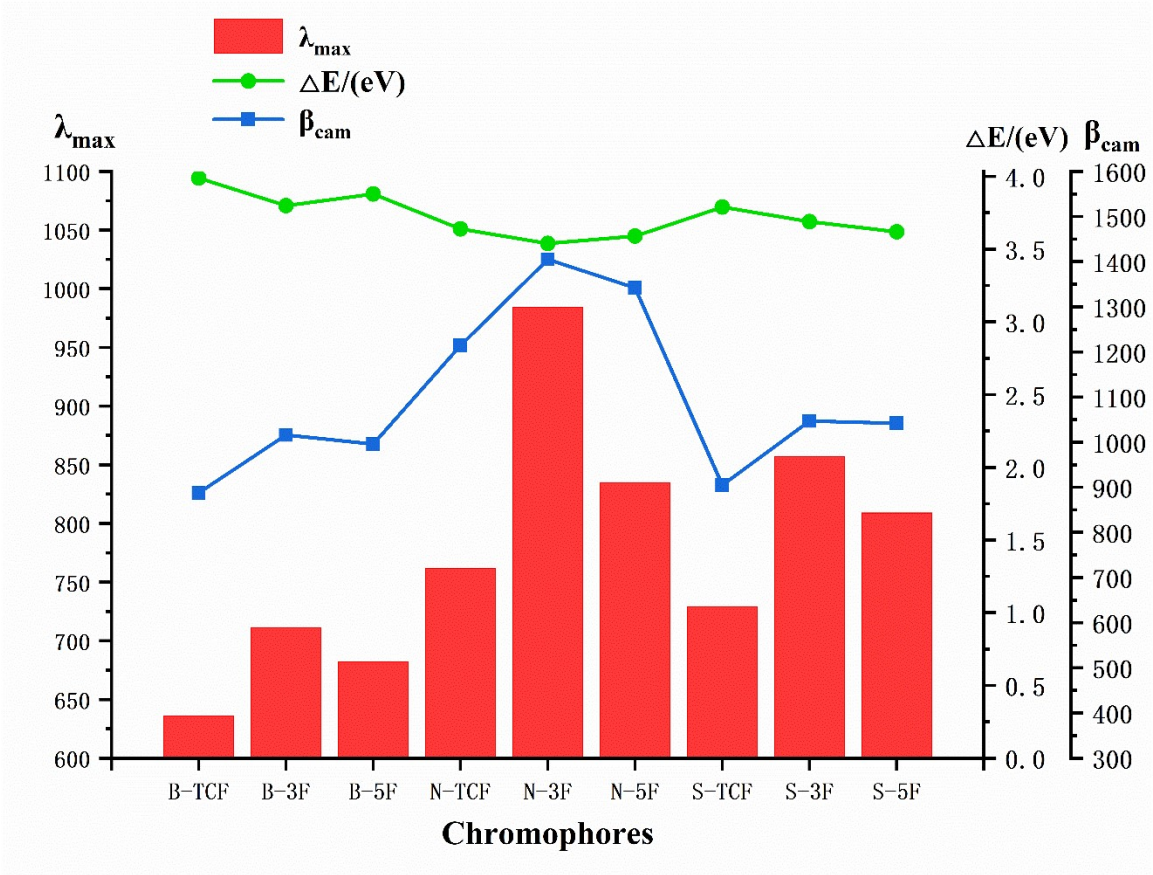

Figure S2. The relationship between λ_{max} 、△E and β_{cam} of the nine chromophores

3. Properties of similar organic EO materials

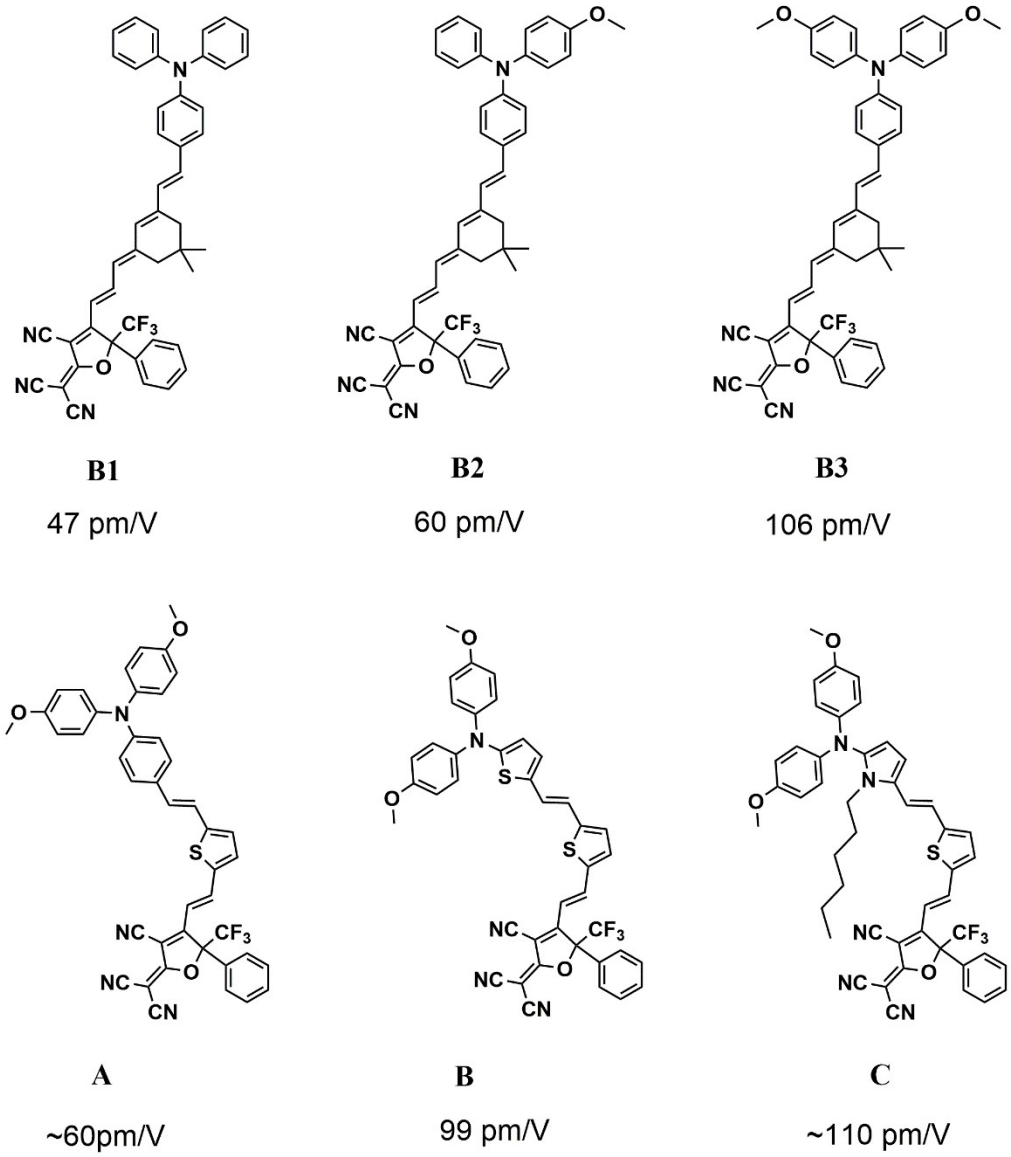

Figure S3. Chemical structures of the similar organic EO materials.[1, 2]

Supplementary Table S3 summarizes the properties of the reported similar organic EO materials, including the chromophore B1-B3 with triphenylamine as the donor and the chromophore A-C with thiophene derivatives as the donor. The chromophores B-3F and S-3F have very similar structures to the reported chromophores B1 and B, and their electro-optical coefficients were also similar. Compared to chromophore B1, chromophore B-3F had a larger electro-optic coefficient, mainly due to the steric hindrance groups on the electron bridge. The N series of chromophores in this paper had a larger electro-optic coefficient than the reported chromophores A-C, because the N series of isophorone electron bridges on N series of chromophores have better electron transfer ability than thiophene bridges, resulting in a larger first-order hyperpolarizability.

4. NMR pictures

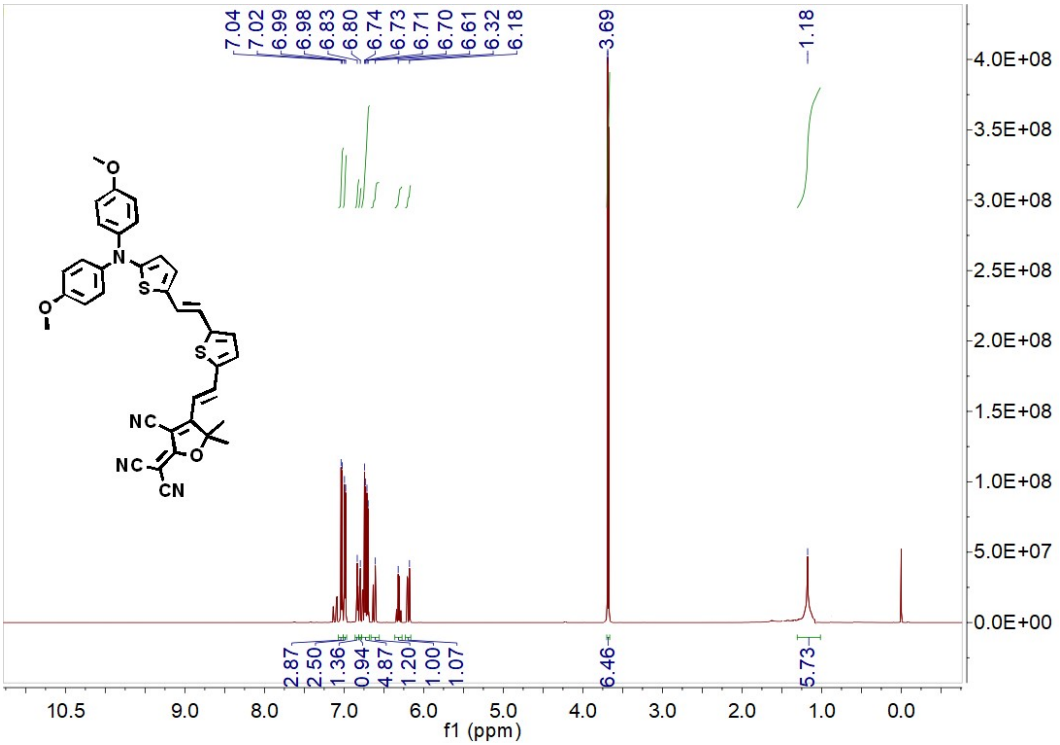

Figure S4. ^{1}H-NMR spectrum of S-TCF.

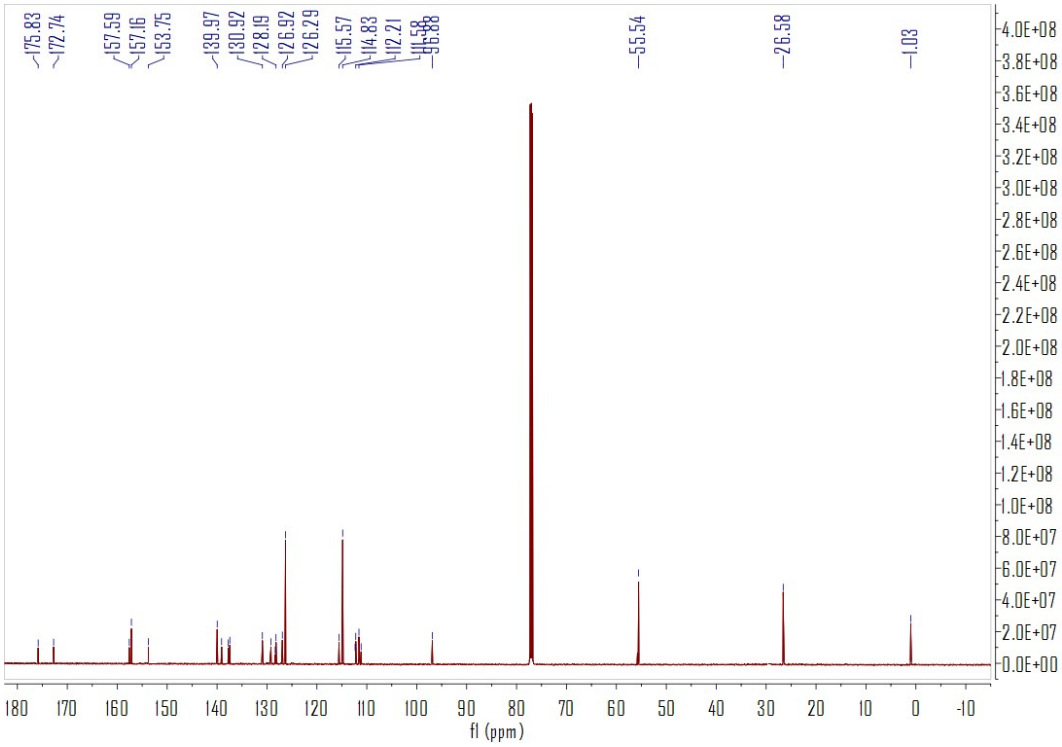

Figure S5. ^{13}C-NMR spectrum of S-TCF.

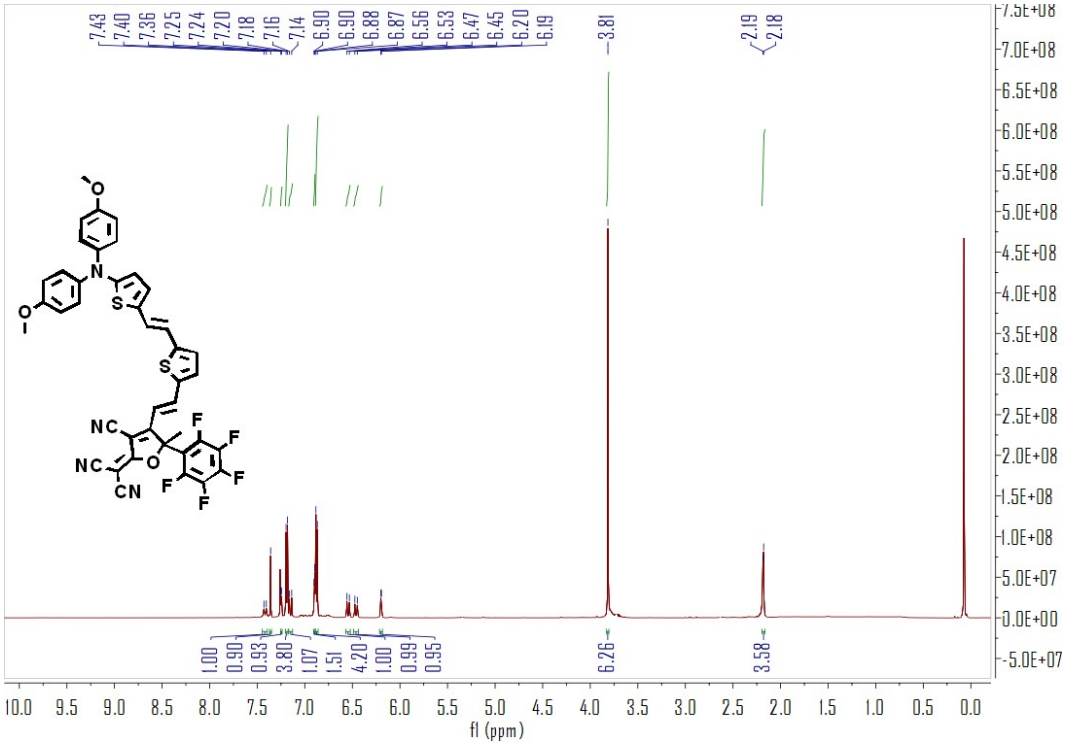

Figure S6. ^{1}H-NMR spectrum of S-5F.

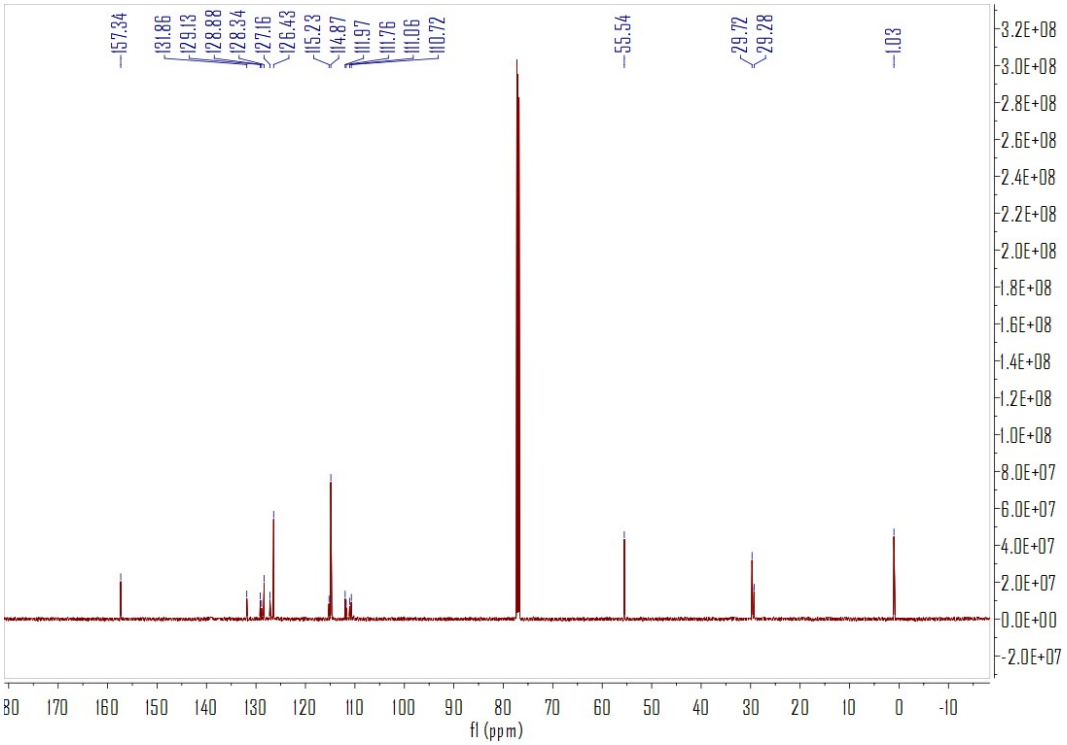

Figure S7. ^{13}C-NMR spectrum of S-5F.

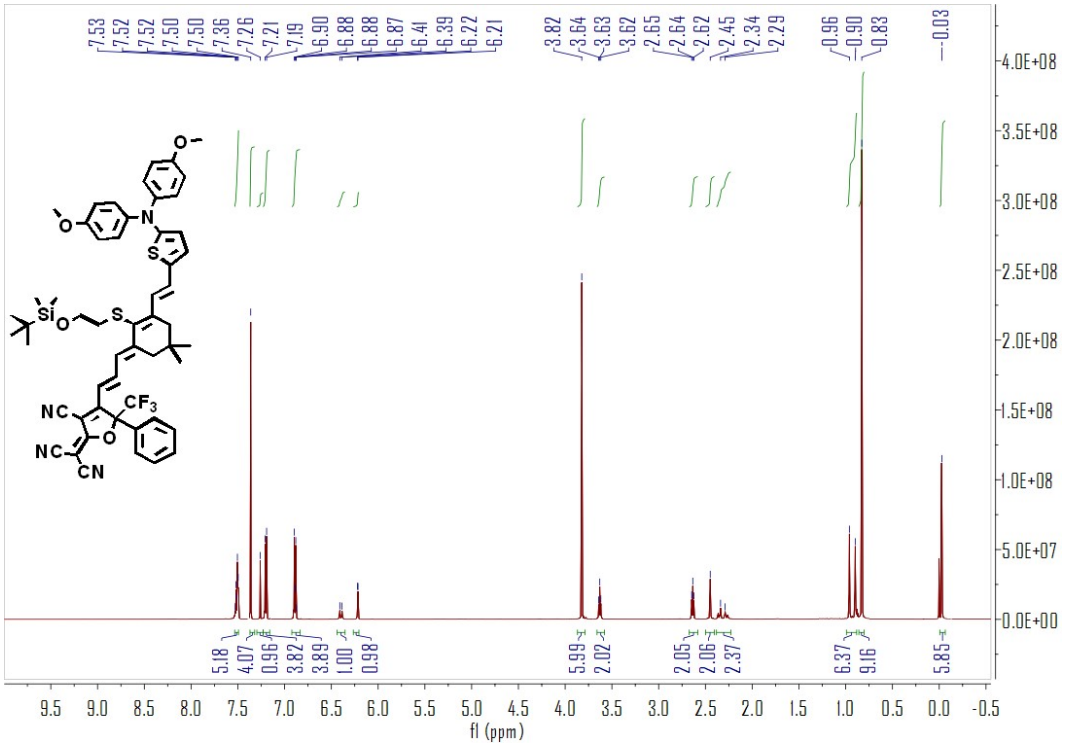

Figure S8. ^{1}H-NMR spectrum of N-3F.

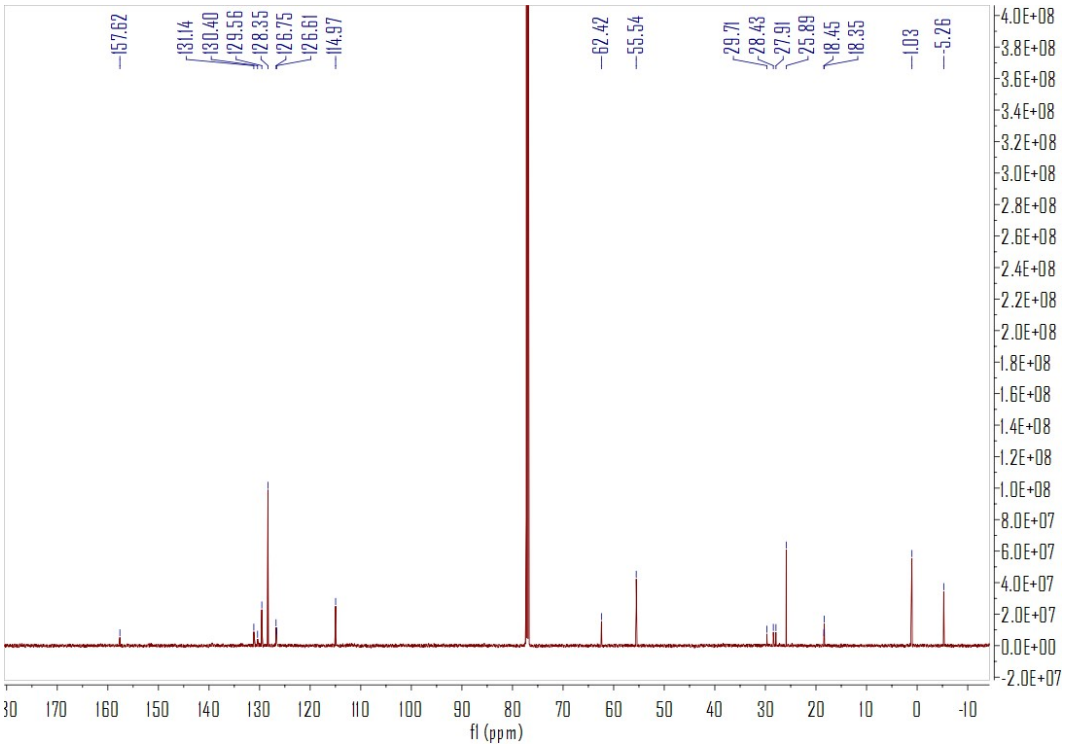

Figure S9. ^{13}C-NMR spectrum of N-3F.

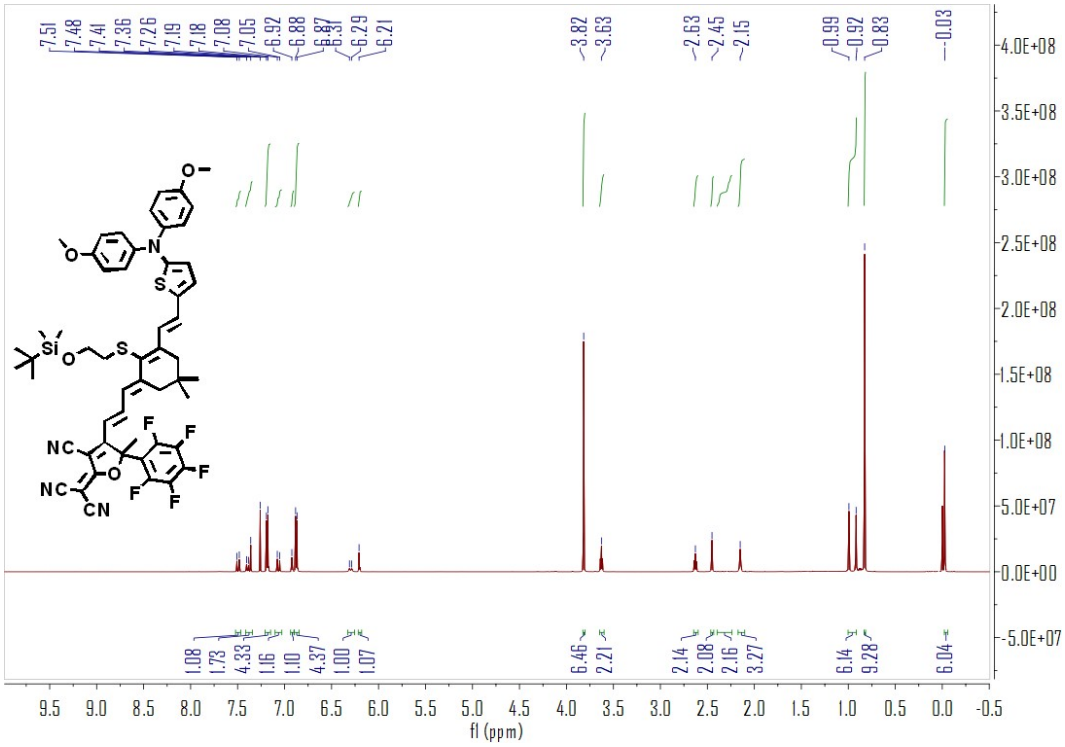

Figure S10. ^{1}H-NMR spectrum of N-5F.

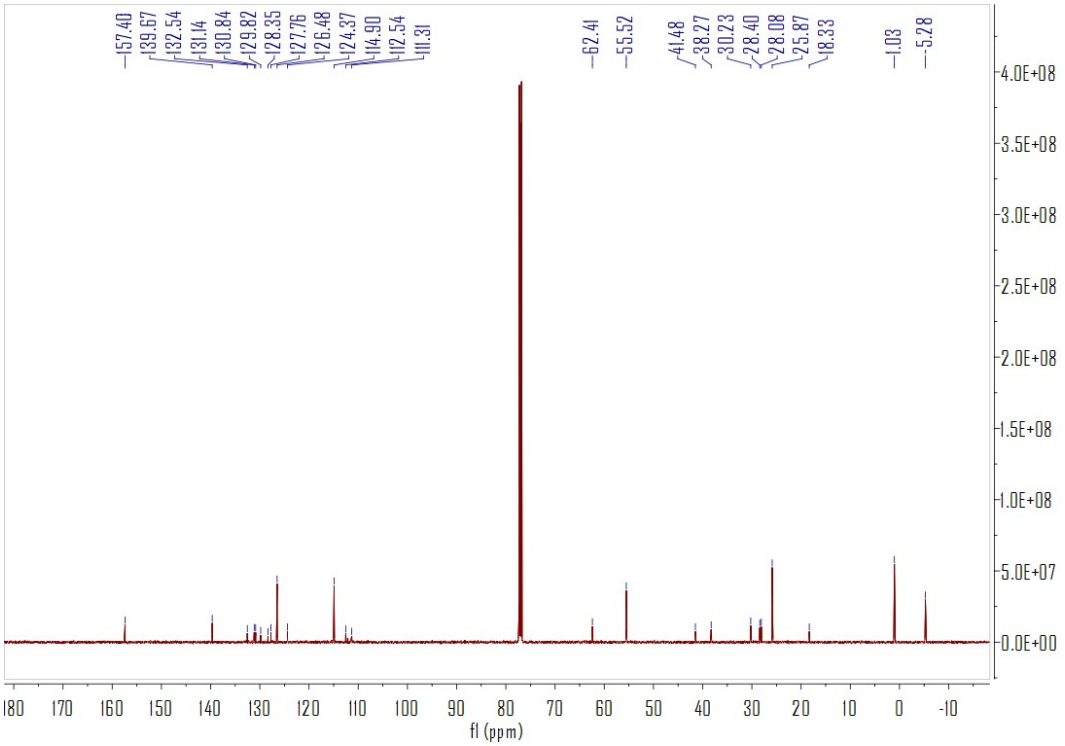

Figure S11. ^{13}C-NMR spectrum of N-5F.

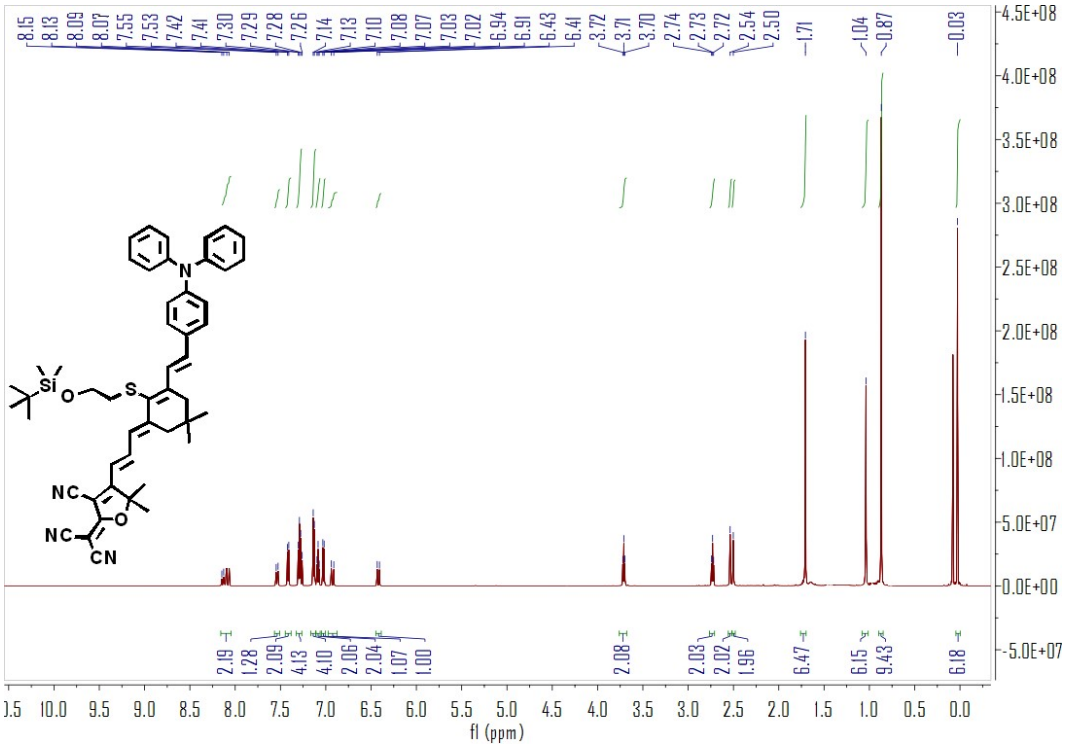

Figure S12. ^{1}H-NMR spectrum of B-TCF.

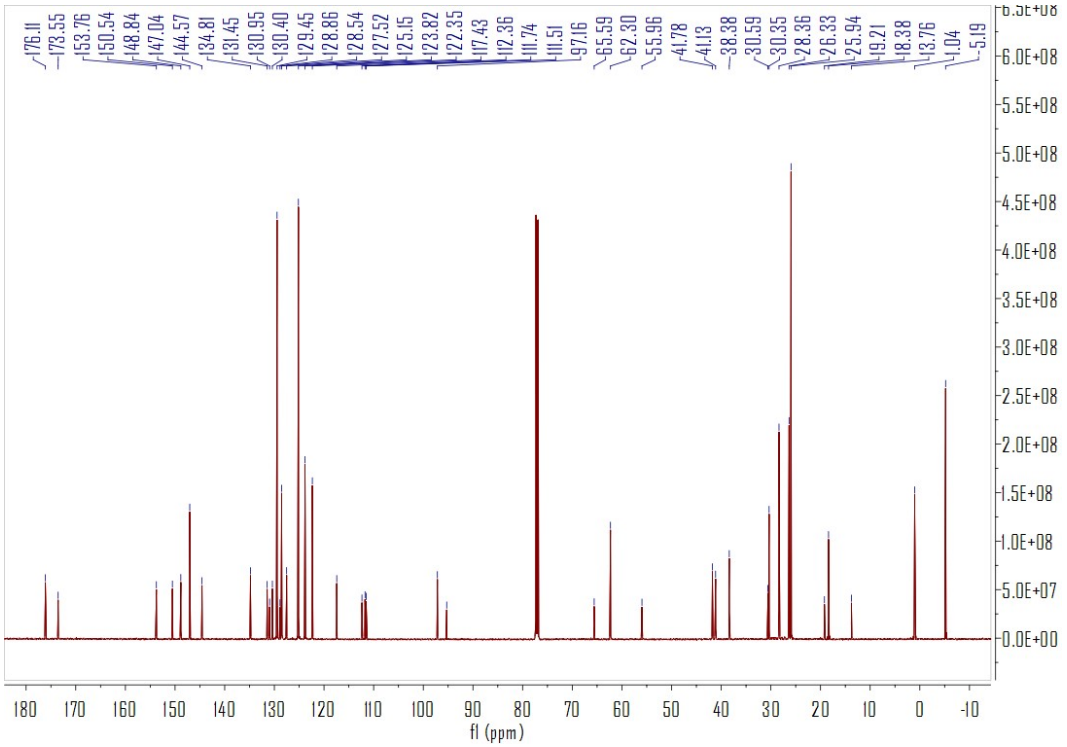

Figure S13. ^{13}C-NMR spectrum of B-TCF.

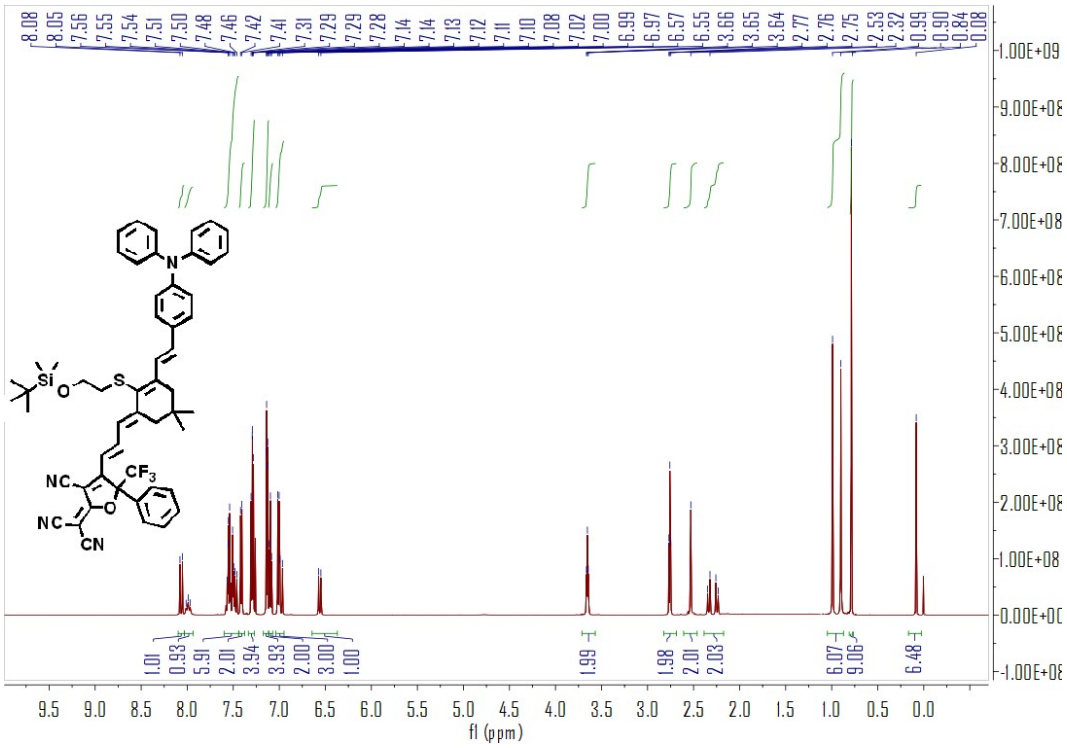

Figure S14. ^{1}H-NMR spectrum of B-3F.

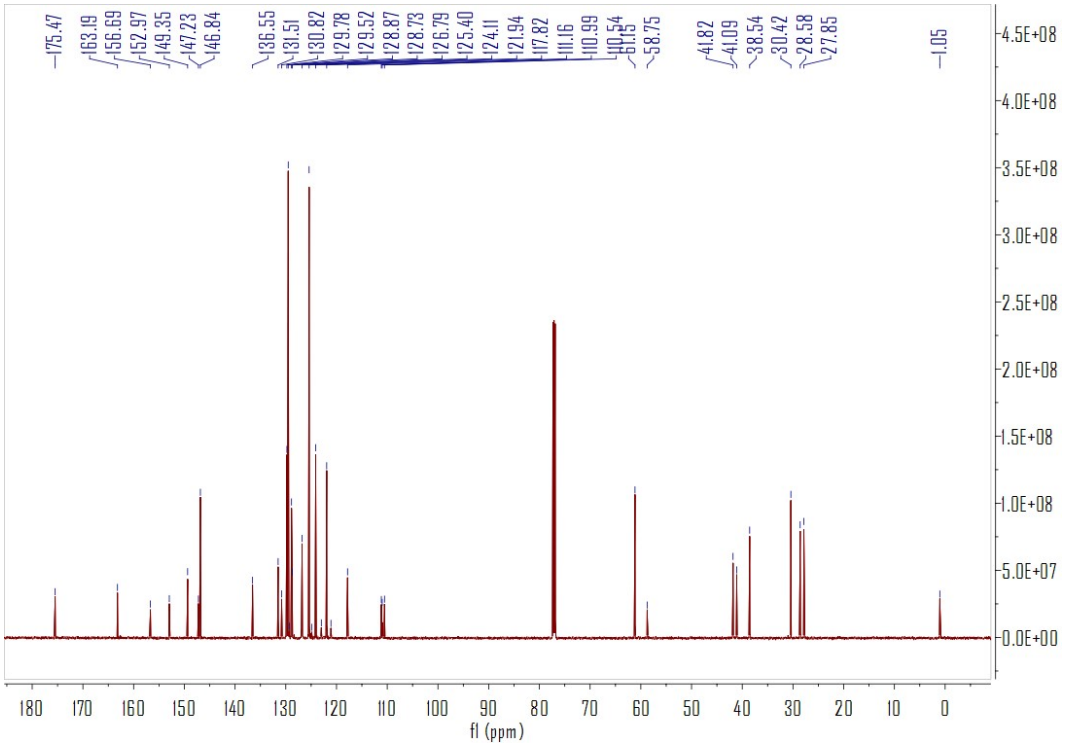

Figure S15. ^{13}C-NMR spectrum of B-3F.

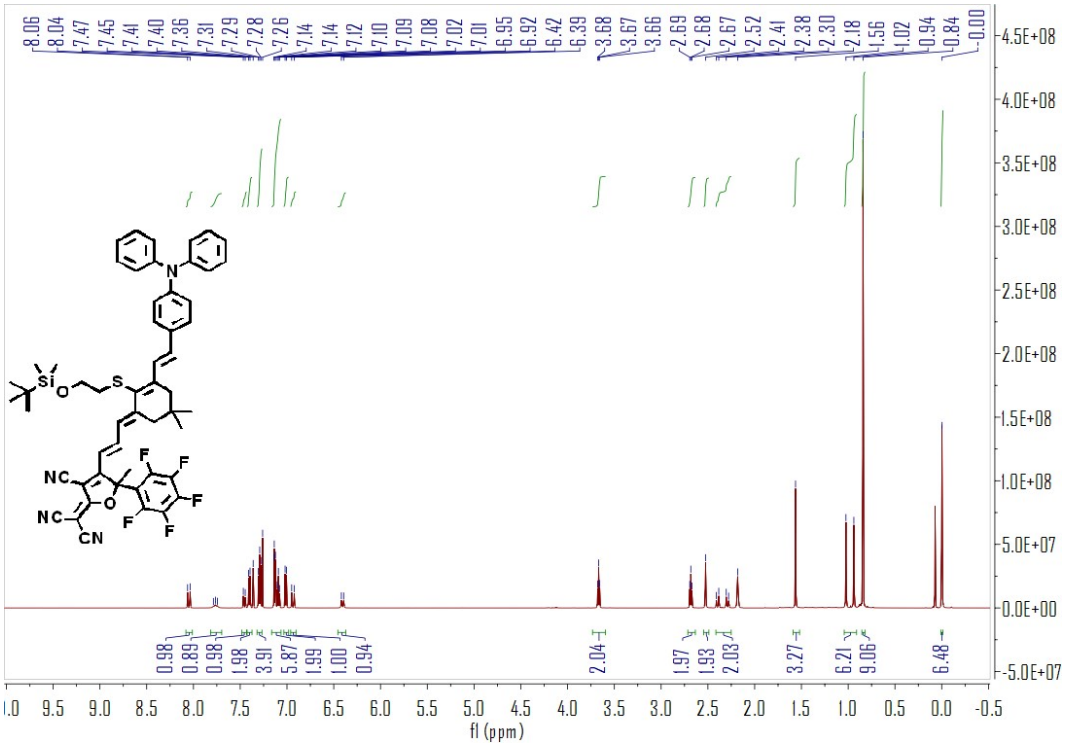

Figure S16. ^{1}H-NMR spectrum of B-5F.

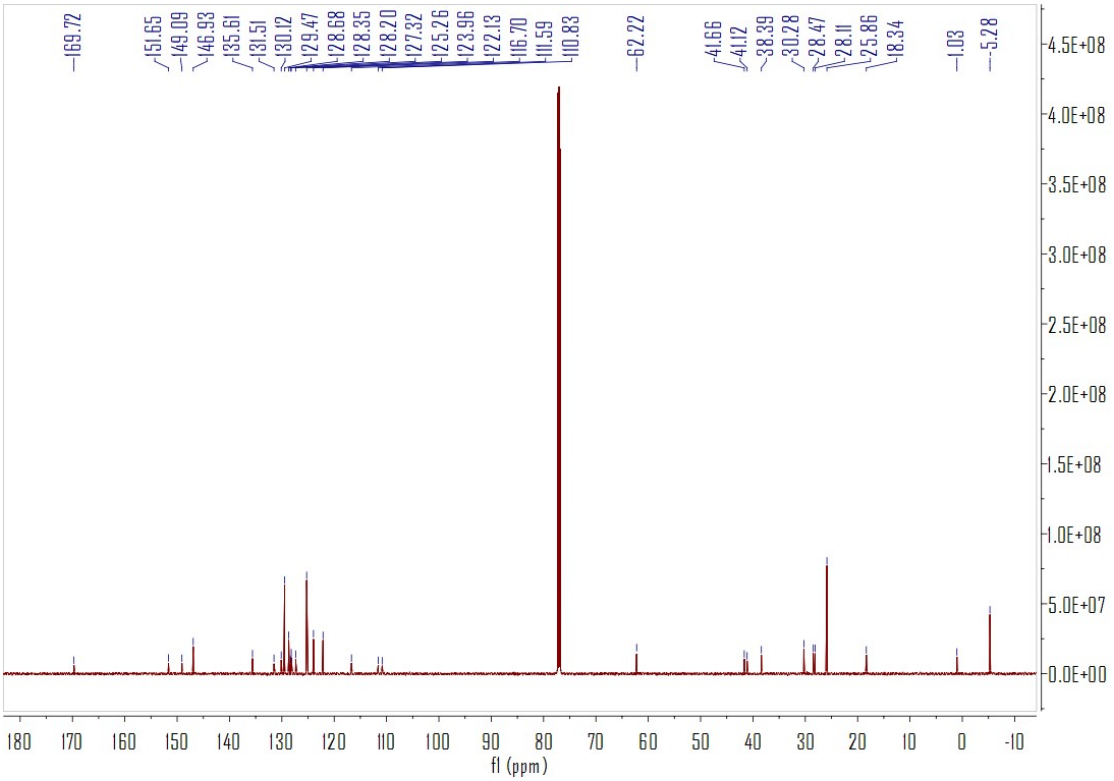

Figure S17. ^{13}C-NMR spectrum of B-5F.

5. References

1. J. A. Davies, A. Elangovan, P. A. Sullivan, B. C. Olbricht, D. H. Bale, T. R. Ewy, C. M. Isborn, B. E. Eichinger, B. H. Robinson, P. J. Reid, X. Li and L. R. Dalton, *Journal of the American Chemical Society*, 2008, **130**, 10565-10575.
2. Y.-J. Cheng, J. Luo, S. Hau, D. H. Bale, T.-D. Kim, Z. Shi, D. B. Lao, N. M. Tucker, Y. Tian, L. R. Dalton, P. J. Reid and A. K. Y. Jen, *Chemistry of Materials*, 2007, **19**, 1154-1163.