

Supplementary Information for

Benzobis(thiadiazole)-Based Small Molecule as a Solution-Processing Electron Extraction Material in Planar Perovskite Solar Cells

*Liping Zhu^{a†}, Changjian Song^{ab†}, Xiaodong Li^a, Ying-Chiao Wang^a, Wenxiao Zhang^{ab}, Xiaohua Sun^c,
Wenjun Zhang^{ab,*} and Junfeng Fang^{ab,*}*

^aKey Laboratory of Graphene Technologies and Applications of Zhejiang Province, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo, 315201, China;

^bUniversity of Chinese Academy of Sciences, Beijing 100049, China

^cCollege of Materials and Chemical Engineering, China Three Gorges University, Yichang 443002, China

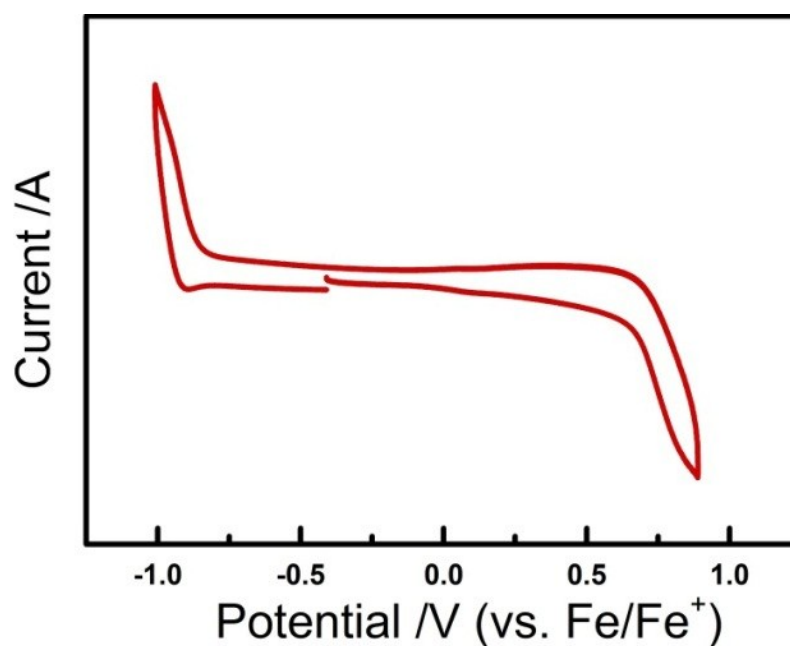


Fig. S1 Cyclic voltammogram of B2F.

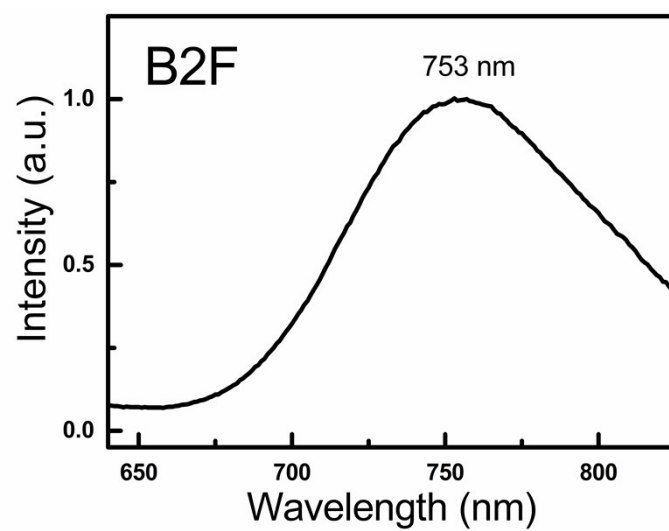


Fig. S2 The PL spectrum of the B2F film.

Table S1 Optical and electrochemical properties of B2F.

Compound	$\lambda_{\text{Abs,max}}$ (solution) (nm)	$\lambda_{\text{Abs,max}}$ (film) (nm)	$E_{\text{g}}^{\text{opt}}$ (eV)	E_{g}^{CV} (eV)	HOMO^{CV} (eV)	LUMO^{CV} (eV)	HOMO^{UPS} (eV)	LUMO^{UPS} (eV)
B2F	345, 615	352, 648	1.65	1.55	-5.49	-3.94	-5.67	-4.02

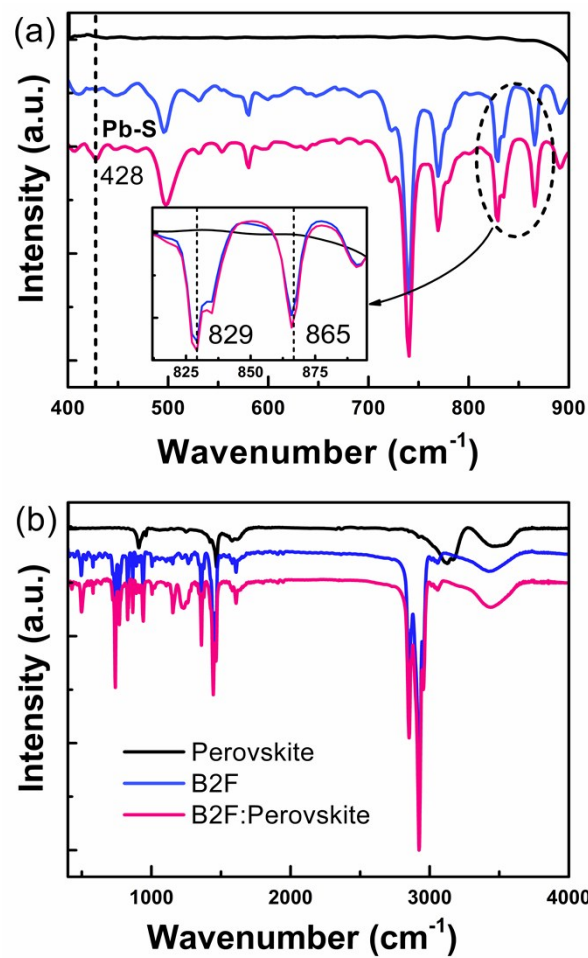


Fig. S3 FTIR of the powders of $\text{CH}_3\text{NH}_3\text{PbI}_3$, B2F, and B2F: $\text{CH}_3\text{NH}_3\text{PbI}_3$ blend. (a) The wavenumber range from 400-900 cm^{-1} . (b) The wavenumber range from 400-4000 cm^{-1} .

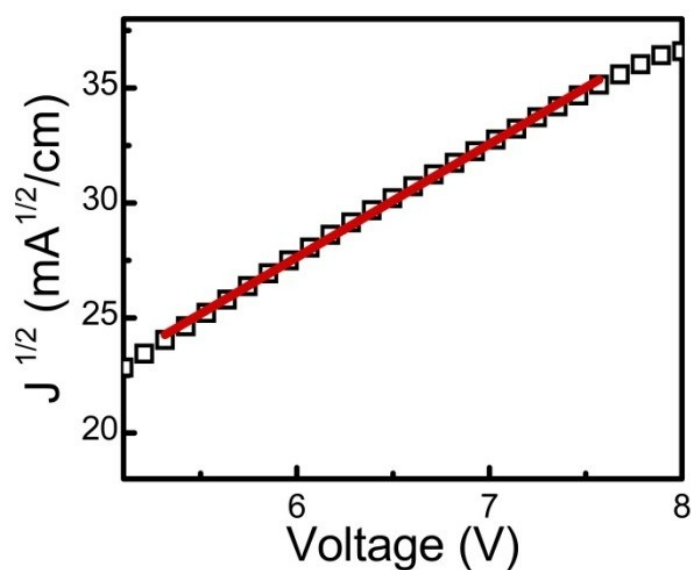


Fig. S4 $J^{1/2}$ - V curve of the electron-only device. The red line represents the linear fitting of the curve at the $n=2$ region.

Table S2 Summary of the device performance determined by forward and reverse scans.

ETL	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE (%)
B2F forward	0.927	19.05	69.90	12.35
B2F reverse	0.920	18.39	64.52	10.92
C ₆₀ forward	1.028	19.58	76.30	15.35
C ₆₀ reverse	1.007	19.60	72.92	14.40
B2F/C ₆₀ forward	1.052	20.63	79.15	17.18
B2F/C ₆₀ reverse	1.049	20.67	78.19	16.96

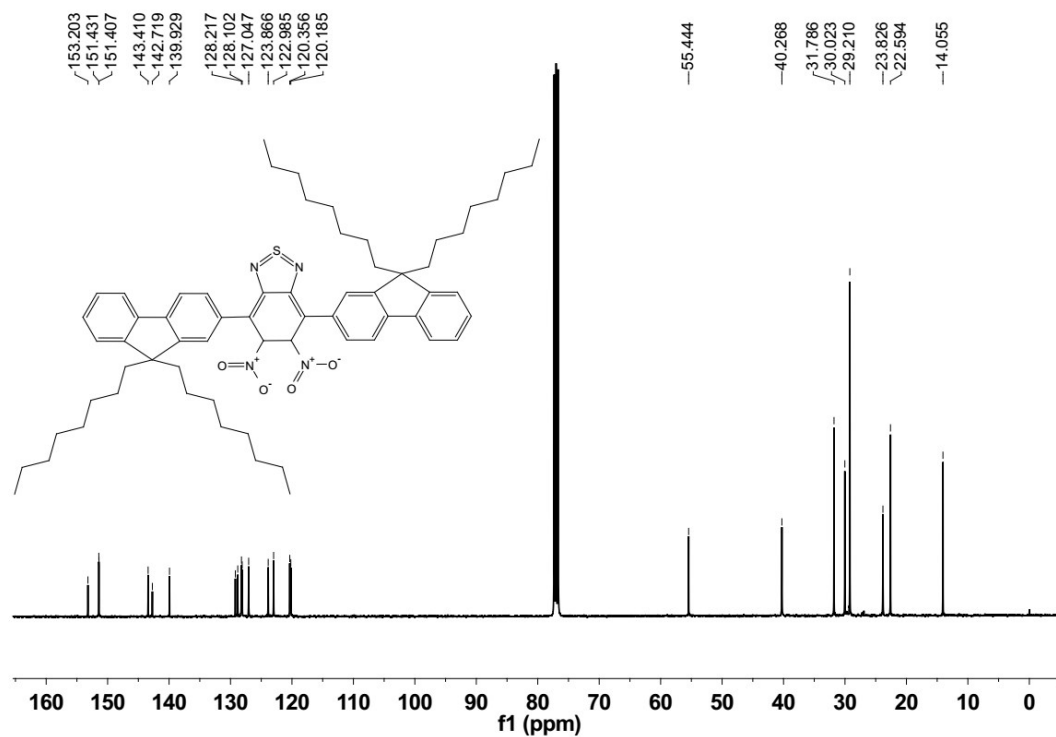


Fig. S5 The ¹³C NMR spectrum of 4,7-bis(9,9-dioctyl-9H-fluoren-2-yl)-5,6-dinitrobenzo[c][1,2,5]thiadiazole.

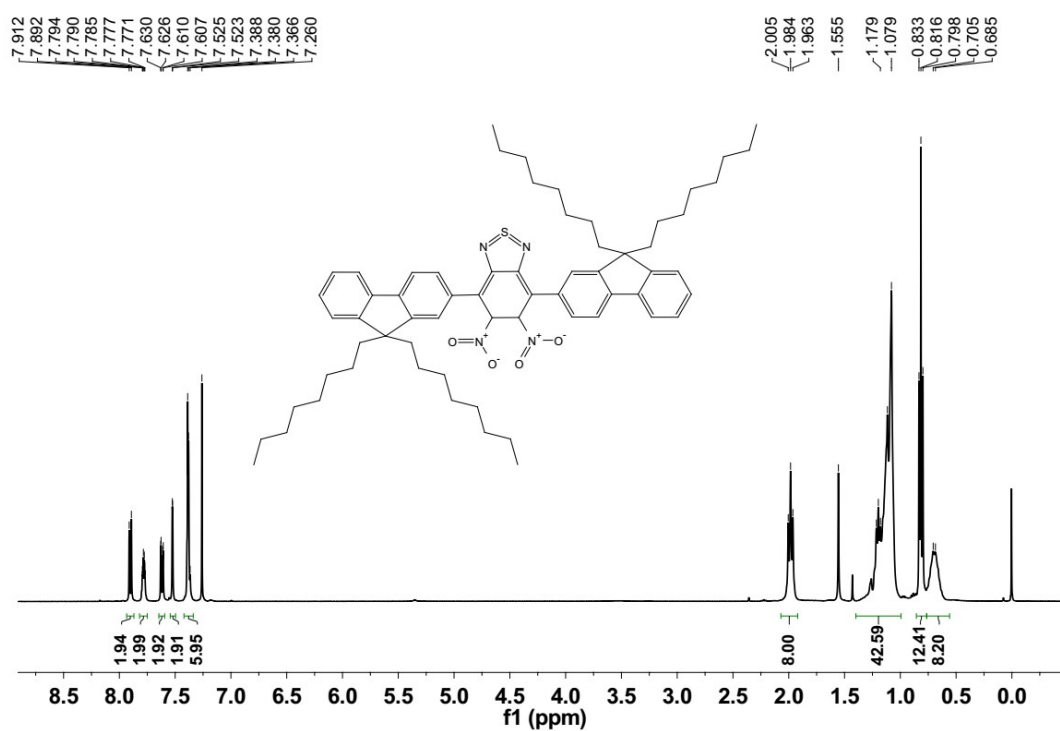


Fig. S6 The ¹H NMR spectrum of 4,7-bis(9,9-dioctyl-9H-fluoren-2-yl)-5,6-dinitrobenzo[c][1,2,5]thiadiazole.

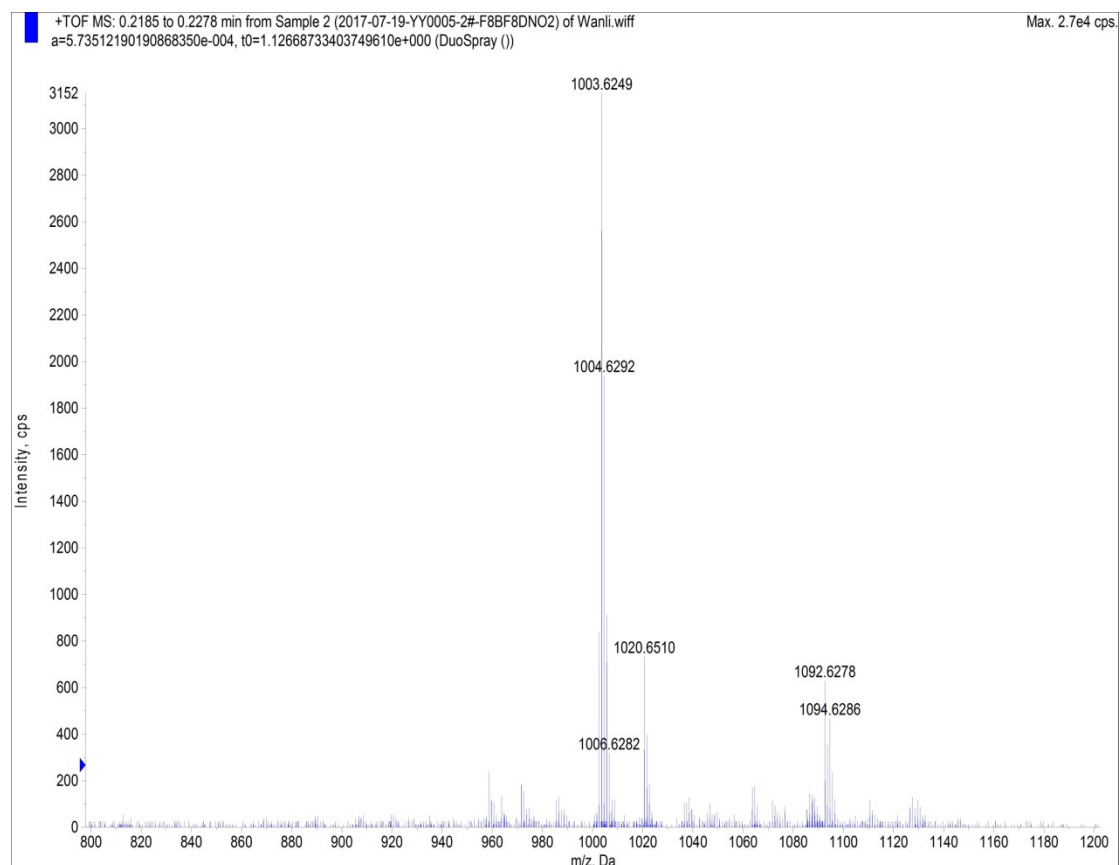


Fig. S7 The HRMS m/z of 4,7-bis(9,9-dioctyl-9H-fluoren-2-yl)-5,6-dinitrobenzo[c][1,2,5] thiadiazole.

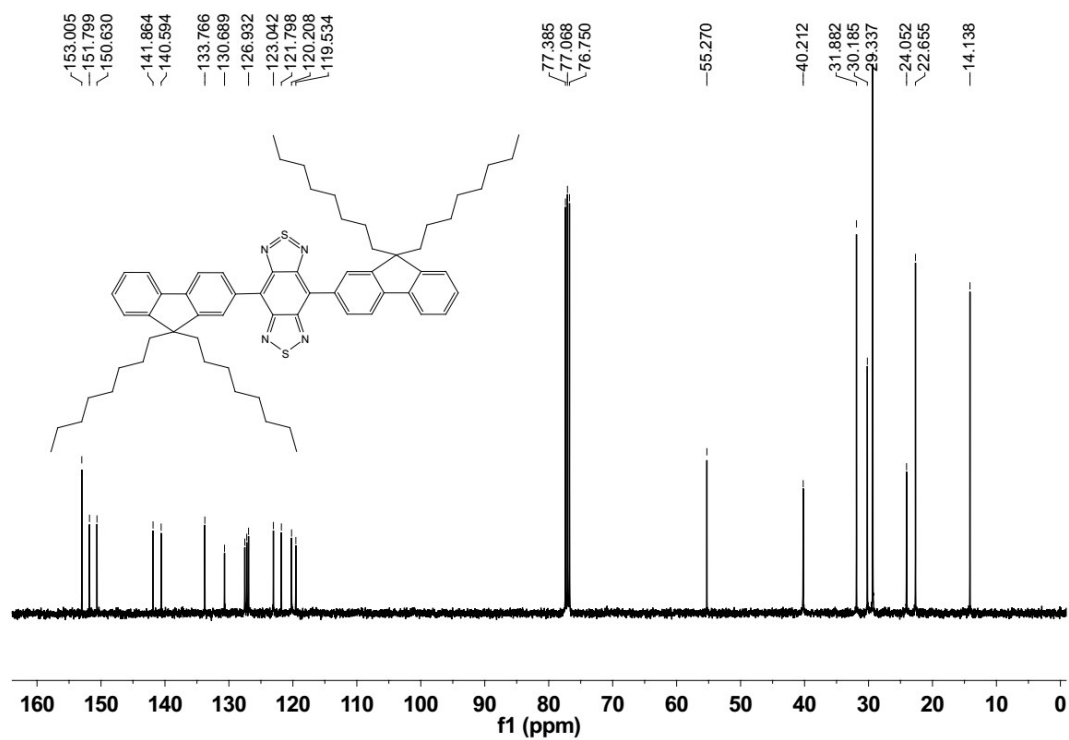


Fig. S8 The ¹³C NMR spectrum of B2F.

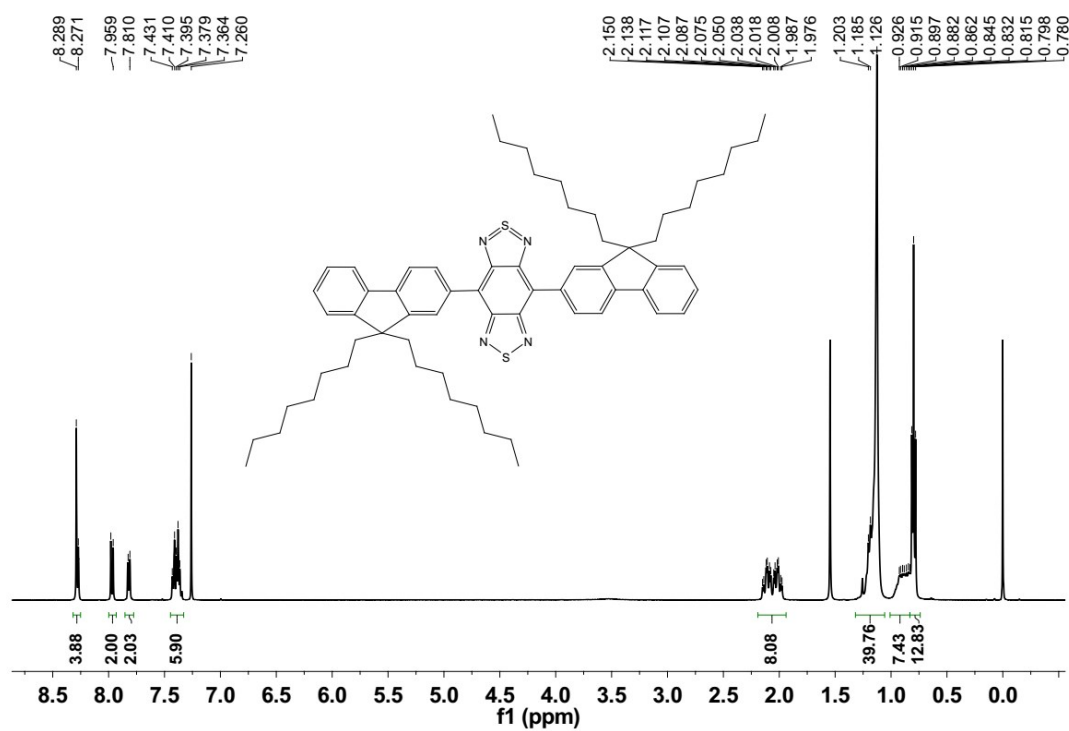


Fig. S9 The ^1H NMR spectrum of B2F.

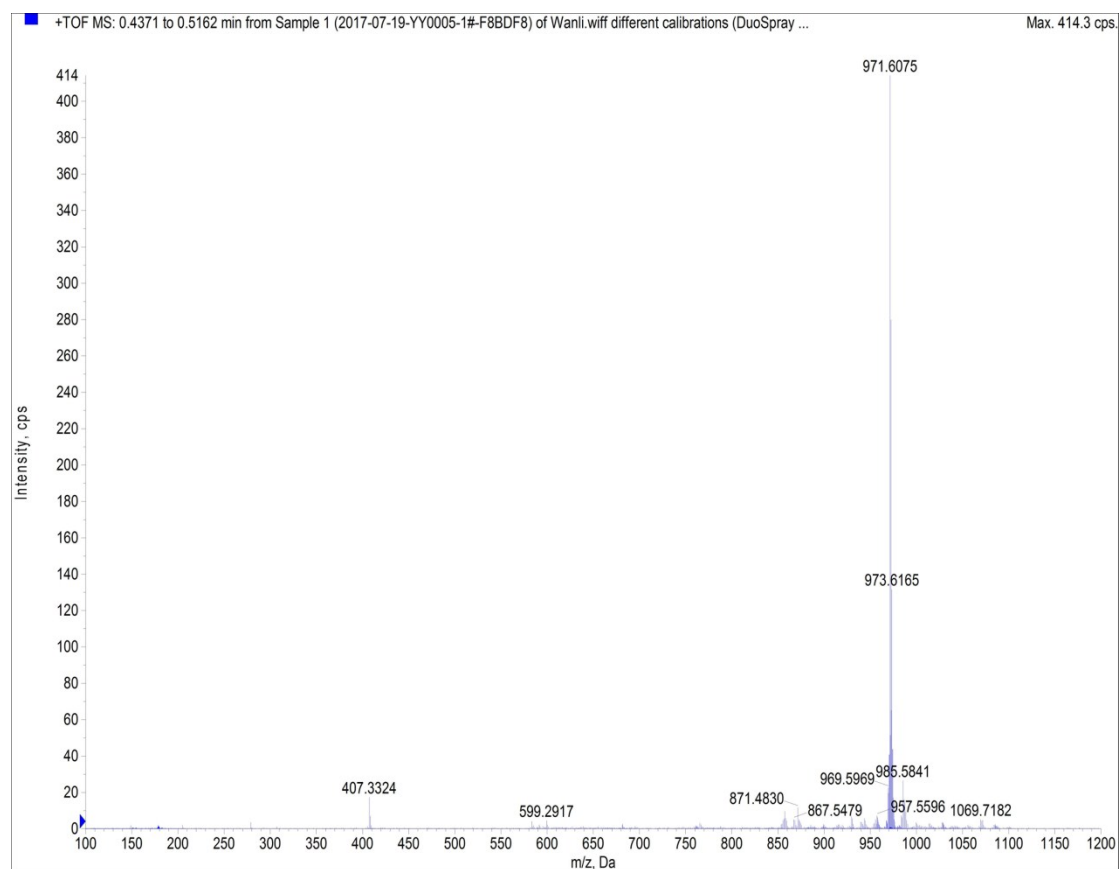


Fig. S10 The HRMS (m/z) of B2F.