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## **Supporting information**

# Synthesis of Largely $\pi$ -Extended Naphthalenediimides via C-H Activation towards Highly Soluble and Narrow Band-Gap Organic

## **Optoelectronic Materials**

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#### **Experimental Section**

#### 1. Materials and General Methods.

Trans-bis(benzonitrile) dichloropalladium  $(PdCl_2(PhCN)_2),$ Tetrakis(triphenylphosphine)palladiuM(0) (Pd(PPh<sub>3</sub>)<sub>4</sub>) were purchased from Aldrich and used without further purification. Other reagents were obtained commercially and used as received. DTYM-NDI-DTYA  $(9)^1$  and NDI-DTYA2  $(8)^2$  were synthesized according to the reported procedures. <sup>1</sup>H NMR (400 MHz) and <sup>13</sup>C NMR (100 MHz) spectra were measured on on JOEL NMR instruments, using tetramethylsilane as an internal standard. MALDI-TOF spectra were carried out on InoSpec 4.7 Tesla FT-MS. Elemental analyses were performed on an Elementa Vario EL III elemental analyzer. FT-IR spectra were determined using a Bio-Rad FTS-185 spectrometer. Absorption spectra were measured on a on a JASCO V-570 UV-vis-NIR spectrophotometer. Thermogravimetric measurements (TGA) were carried out on a TA Q500 instruments under a dry nitrogen flow at a heating rate of 10 °C/min, heating from room temperature to 500 °C. Differential scanning calorimetry (DSC) analysis was performed on a Perkin Elmer Pyris I instruments under nitrogen atmosphere at a heating (cooling) rate of 10 °C/min. The first cooling and second heating DSC scans are recorded. Cyclic voltammetric measurements were carried out in a conventional three-electrode cell using a platinum button working electrode of 2 mm diameter, a platinum wire counter electrode, and a saturated calomel electrode (SCE) reference electrode on a computer-controlled CHI610D instruments (ferrocene as the internal standard,  $E_{\text{Fc+/Fc}} = 0.36 \text{ V}$ ). X-ray diffraction (XRD) data were collected from an X'Pert Pro diffraction instrument. AFM images were recorded on a Nanoscope Iva-Multimode atomic force microscope in tapping mode.

#### 2. OTFT Device Fabrication and Measurements.

An n-type heavily doped Si wafer with a SiO<sub>2</sub> layer of 300 nm and a capacitance of 11 nF/cm<sup>2</sup> was used as the gate electrode and dielectric layer. Thin films (25–40 nm in thickness) of semiconductors **4** were deposited on octadecyltrichlorosilane (OTS)-treated SiO<sub>2</sub>/Si substrates by spin-coating their respectively solutions (10 mg/mL). Then, the thin films were annealed at different temperatures for improving their thin-film quality/morphology. Gold source and drain contacts (50 nm in thickness) were deposited by vacuum evaporation on the organic layer through a shadow mask, affording a bottom-gate top-contact device configuration. The channel width (W) /length (L) = 8.95. Electrical measurements of OTFT devices were carried out at room temperature in air using a Keithley 4200 semiconductor parameter analyzer. The field-effect mobility was calculated in the saturation regime by using the equation  $I_{DS}$ = ( $\mu WC_i/2L$ )( $V_G - V_T$ )<sub>2</sub>, where  $I_{DS}$  is the drain-source current,  $\mu$  is the field-effect mobility. W is the channel width (237 µm), L is the channel length (31 µm), C<sub>i</sub> is the capacitance per unit area ( 9.8 nF) of the gate dielectric layer, V<sub>G</sub> is the gate voltage, and V<sub>T</sub> is the threshold voltage.

#### 3. Synthesis and characterization.



7. To a solution of **1** (400 mg, 0.343 mmol) in CHCl<sub>3</sub> (30 mL), Br<sub>2</sub> (60 mg, 0.378 mmol) in 30 mL CHCl<sub>3</sub> was added dropwise at room temperature, and the mixture was stirred for 2 hours. The solvent was then removed under reduced pressure. The residue was purified by chromatography with dichloromethane/petroleum ether (1/2) as eluent. Compound **2** was obtained as blue solid, 230 mg (yield, 54%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, mixture of Z/E)  $\delta$  0.85–0.88 (m, 12H, –CH<sub>3</sub>), 1.22 (br, 80H, – CH<sub>2</sub>–), 1.99 (br, 2H, –CH–), 4.15–4.17 (m, 4H, –CH<sub>2</sub>–N), 5.68 (s, 1H, =CH–CN).; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, mixture of Z/E):  $\delta$ : 14.26 22.83, 26.47, 29.52, 29.76, 29.83, 30.19, 30.23, 31.64, 32.07, 36.58, 36.63, 46.20, 46.30, 71.07, 85.40, 114.40, 115.69, 115.94, 116.05, 116.23, 124.79, 125.08, 144.80, 146.94, 147.03, 161.87, 162.13, 162.18, 162.31, 164.60; MS (MALDI-TOF) m/z: 1323.3 M<sup>+</sup>; MS (MALDI-TOF) m/z: 1244.0 (M+H)<sup>+</sup>; HR-MS: (MALDI/DHB) Calcd. For C<sub>74</sub>H<sub>104</sub>O<sub>4</sub>N<sub>4</sub>S<sub>4</sub>: 1243.5805, Found: 1243.5863.

**3a**. Under a nitrogen atmosphere, a mixture of **2** (200 mg, 0.161 mmol), (4-(trifluoromethyl)phenyl)boronic acid (51 mg, 0.402 mmol), Pd(PPh<sub>3</sub>)<sub>4</sub> (19 mg, 0.016 mmol), and K<sub>2</sub>CO<sub>3</sub> (133 mg, 1.288 mmol) in 20 mL redistilled THF and 2 mL H<sub>2</sub>O was stirred at 100 °C for 10 h. The mixture was poured into methanol after refluxing 10 hours. The blue precipitate was filtered and purified by chromatography with

dichloromethane/petroleum ether (1/2) as eluent. Compound **3a** was obtained as blue solid, 177mg in 77% yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, mixture of Z/E)  $\delta$ 7.82 (br, 4H, =CH–), 5.65 (br, 1H, =CH–CN), 4.17–4.12 (br, 4H, –CH<sub>2</sub>–N), 1.98, 1.97 (br, 2H, – CH–), 1.23 (m, 80H, –CH<sub>2</sub>–), 0.86, 0.85 (m, 12H, –CH<sub>3</sub>). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  162.13, 161.17, 160.37, 156.00, 146.81, 133.21, 127.88, 127.17, 126.62, 125.15, 124.99, 118.79, 115.97, 114.89, 100.11, 94.16, 85.13, 79.15, 66.01, 46.08, 38.69, 36.57, 36.43, 34.82, 32.01, 31.62, 31.52, 31.15, 30.13, 29.77, 29.74, 29.45, 28.46, 26.41, 24.21, 22.77, 19.12, 14.20; MS (MALDI-TOF) m/z: 1309.5 (M+H)<sup>+</sup>; HR-MS: (MALDI/DHB) Calcd. For C<sub>75</sub>H<sub>103</sub>F<sub>3</sub>O<sub>4</sub>N<sub>4</sub>S<sub>4</sub>: 1309.6887, found: 1309.6876.

The same procedure was followed for the synthesis of compounds **3b** and **3c**, using phenylboronic acid and (4-(diphenylamino)phenyl)boronic acid instead of (4-(trifluoromethyl)phenyl)boronic acid, respectively.

**3b** was obtained as blue solid in 89% yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, mixture of Z/E)  $\delta$  7.67, 7.65 (d, 2H, =CH–), 7.56, 7.54, 7.52 (t, 2H, =CH–), 7.47, 7.45, 7.44 (t, 1H, =CH–), 5.62 (s, 1H, =CH–CN), 4.15–4.10 (br, 4H, –CH<sub>2</sub>–N), 1.97 (br, 2H, –CH–), 1.22 (m, 80H, –CH<sub>2</sub>–), 0.86 (m, 12H, –CH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  164.8, 162.24, 162.12, 157.38, 147.37, 147.30, 146.62, 146.51, 146.41, 146.29, 146.02, 145.94, 132.90, 129.59, 127.43, 124.89, 115.82, 101.96, 84.78, 46.08, 35.56, 36.41, 32.02, 31.59, 31.51, 30.17, 29.80, 29.77, 29.48, 26.48, 26.42, 22.79, 14.23; MS (MALDI-TOF) m/z: 1241.7 (M+H)<sup>+</sup>; HR-MS: (MALDI/DHB) Calcd. For C<sub>74</sub>H<sub>104</sub>O<sub>4</sub>N<sub>4</sub>S<sub>4</sub>: 1241.7013, found: 1241.6994.

**3c** was obtained as blue solid in 98% yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, mixture of Z/E) δ 7.39–7.35 (m, 6H, =CH–), 7.24, 7.22 (d, 4H, =CH–), 7.18, 7.16, 7.14 (t, 2H, =CH–), 7.09, 7.07 (br, 2H, =CH–), 5.55 (br, 1H, =CH–CN), 4.13–4.12 (br, 4H, – CH<sub>2</sub>–N), 2.00 (br, 2H, –CH–) 1.23 (m, 80H, –CH<sub>2</sub>–), 0.86 (m, 12H, –CH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 164.91, 162.16, 162.02, 161.91, 148.79, 146.64, 146.26, 146.05, 145.82, 129.75, 128.03, 125.98, 124.98, 124.58, 121.08, 116.80, 115.80, 115.36, 115.09, 102.02, 84.43, 77.44, 77.12, 76.80, 46.23, 36.54, 36.37, 32.02, 31.62, 31.52, 30.22, 29.79, 29.47, 26.51, 26.45, 22.78, 14.21; MS (MALDI-TOF) m/z: 1408.8 (M+H)<sup>+</sup>; HR-MS: (MALDI/DHB) Calcd. For C<sub>86</sub>H<sub>113</sub>O<sub>4</sub>N<sub>5</sub>S<sub>4</sub>: 1408.7748, found:

S5

1408.7738.

**4a**. Under a nitrogen atmosphere, a mixture of **3a** (40 mg, 0.03 mmol),  $PdCl_2(PhCN)_2$  (0.35 mg, 0.09% mmol), AgNO<sub>3</sub> (20.4 mg, 0.12 mmol), and KF (7.0 mg, 0.12 mmol) in 2 mL DMF was stirred at 120 °C for 3 hours. The mixture was poured into methanol. The green precipitate was filtered and purified by column chromatography, using dichloromethane/petroleum ether (1/2) as the eluent. 32.8 mg of green **4a** was obtained as green solid (yield, 85%). M.p.: 300 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, mixture of Z/E)  $\delta$  7.82 (br, 8H, =CH–), 4.25–4.11 (br, 8H, –CH<sub>2</sub>–N), 2.02 (br, 4H, – CH–), 1.24–1.18 (m, 160H, –CH<sub>2</sub>–), 0.86–0.83 (m, 24H, –CH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  162.24, 160.38, 147.30, 145.84, 136.45, 127.89, 126.65, 125.24, 125.11, 116.91, 116.69, 116.27, 116.10, 113.84, 100.36, 90.56, 77.42, 77.10, 76.78, 46.28, 36.64, 36.51, 32.00, 31.67, 31.57, 31.48, 30.13, 29.75, 29.73, 29.45, 26.42, 22.77, 14.19; MS (MALDI-TOF) m/z: 2616.2 (M+H)<sup>+</sup>; Anal. Calcd. For C<sub>150</sub>H<sub>204</sub>F<sub>6</sub>N<sub>8</sub>O<sub>8</sub>S<sub>8</sub>: C, 68.82; H, 7.85; N, 4.28; found: C, 69.01; H, 7.81; N, 4.19.

The same procedure was followed for the synthesis of compounds **4b** and **4c**, using **3b** and **3c** instead of **3a**, respectively.

**4b** was obtained as green solid (yield, 90%). M.p.: 291 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, mixture of Z/E) δ 7.67–7.65 (br, 4H, =CH–), 7.57–7.53 (m, 4H, =CH–), 7.49–7.44 (m, 2H, =CH–), 4.25–4.11 (m, 8H, –CH<sub>2</sub>–N), 2.01 (m, 4H, –CH–), 1.25–1.18 (m, 160H, –CH<sub>2</sub>–), 0.86–0.83 (m, 24H, –CH<sub>3</sub>); <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>) δ 168.42, 162.31, 157.54, 148.20, 146.89, 145.47, 133.04, 129.58, 127.47, 125.13, 116.93, 115.78, 113.93, 102.26, 90.42, 46.27, 36.49, 31.96, 31.65, 30.09, 29.71, 29.39, 26.44, 26.37, 22.72, 14.10; MS (MALDI-TOF) m/z: 2503.2 (M+Na)<sup>+</sup>; Anal. Calcd. For C<sub>148</sub>H<sub>206</sub>N<sub>8</sub>O<sub>8</sub>S<sub>8</sub>: C, 71.63; H, 8.37; N, 4.52; Found: C, 71.57; H, 8.44; N, 4.29.

**4c** was obtained as green solid (yield, 94%). M.p.: 322 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, mixture of Z/E) δ 7.52–7.49 (m, 4H, =CH–), 7.37–7.31 (m, 8H, =CH–), 7.26–7.19 (m, 8H, =CH–), 7.16–7.10 (m, 8H, =CH–), 4.25–4.10 (br, 8H, –CH<sub>2</sub>–N), 2.01 (br, 4H, –CH–), 1.24-1.17 (m, 160H, –CH<sub>2</sub>–), 0.85 (m, 24H, –CH<sub>3</sub>); <sup>13</sup>C (100 MHz, CDCl<sub>3</sub>) δ 162.31, 148.91, 146.72, 129.71, 128.29, 125.81, 125.36, 125.22, 124.47, 121.38, 102.43, 77.42, 77.10, 76.78, 46.22, 36.48, 32.01, 31.57, 30.14, 29.76, 29.73,

29.46, 26.46, 22.78, 14.21; MS (MALDI-TOF) m/z: 2814.4 (M+H)<sup>+</sup>; Anal. Calcd. For C<sub>172</sub>H<sub>224</sub>N<sub>10</sub>O<sub>8</sub>S<sub>8</sub>: C, 73.36; H, 8.02; N, 4.97; Found: C, 73.51; H, 7.99; N, 4.84.



Scheme S1. Synthesis of (DTYM-NDI-DTYA)<sub>2</sub>

(**DTYM-NDI-DTYA**)<sub>2</sub>. Under a nitrogen atmosphere, a mixture of **5** (40 mg, 0.037 mmol), PdCl<sub>2</sub>(PhCN)<sub>2</sub> (0.43 mg, 0.001 mol), AgNO<sub>3</sub> (25.2 mg, 0.148 mmol), and KF (8.6 mg, 0.148 mmol) in 2 mL DMF was stirred in 120 °C for 3 hours. The mixture was poured into methanol. The green precipitate was filtered and purified by column chromatography, using dichloromethane/petroleum ether (1/2) as the eluent. (**DTYM-NDI-DTYA**)<sub>2</sub> was obtained 33.2 mg (yield, 83%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 4.27–4.17 (m, 8H, –CH<sub>2</sub>–N), 2.04–2.00 (br, 4H, –CH–), 1.27–1.19 (m, 128H, –CH<sub>2</sub>–), 0.88–0.82 (m, 24H, –CH<sub>3</sub>); <sup>13</sup>C (100 MHz, CDCl<sub>3</sub>) δ 182.47, 168.09, 162.20, 162.18, 162.17, 162.13, 147.42, 147.40, 144.42, 144.37, 125.26, 125.13, 117.85, 117.76, 116.77, 113.59, 111.87, 91.30, 70.61, 46.47, 31.99, 29.75, 29.70, 29.63, 29.41, 22.79, 22.77, 14.24, 14.23, 14.21.

#### 4. The HPLC data of 2, (DTYM-NDI-DTYA)<sub>2</sub>, and 4a.





5. Plausible reaction mechanism of homocoupling.



Scheme S2. Plausible reaction mechanism of homocoupling.

#### Reference

1. Y. Hu, Z. Wang, X. Zhang, X. Yang, C. Ge, L. Fu and X. Gao, *Org. Lett.*, **2017**, *19*, 468-471.

2. Z. Zhao, F. Zhang, Y. Hu, Z. Wang, B. Leng, X. Gao, C.-a. Di and D. Zhu, *ACS Macro. Lett.*, **2014**, *3*, 1174.

## 6. TGA and DSC curves for 4a-c.





Figure S5. DSC plots of 4a–c.



#### 7. UV-vis-NIR spectra of 4a–c in solution and thin film.

**Figure S6.** UV-vis-NIR spectra of **4a–c** (red: in CHCl<sub>3</sub> with a concentration of  $2 \times 10^{-5}$  M; blue: as-spun film).

#### 8. Characteristics of OFET devices.

**Table S1**. Average (Maximum) mobilities ( $\mu_e$ ), current on/off ratios ( $I_{on}/I_{off}$ ), and threshold voltages ( $V_T$ ) for thin film of **4a–c** fabricated by spin coating on OTS-treated Si/SiO<sub>2</sub> substrates at different annealing temperatures.

	annealed at 80 °C				annealed at 120 °C			annealed at 160 °C		
	$\mu_{e}^{a}$ (cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup> )	$I_{\rm on}/I_{\rm off}{}^{\rm a}$	$V_{\mathrm{T}^{a}}\left(\mathrm{V}\right)$	$     \mu_e^a     (cm^2 V^{-1}     s^{-1}) $	$I_{\rm on}/I_{\rm off}{}^{\rm a}$	$V_{T}^{a}(V)$	$\mu_{e}^{a}$ (cm <sup>2</sup> V <sup>-</sup> <sup>1</sup> s <sup>-1</sup> )	$I_{\rm on}/I_{\rm off}{}^{\rm a}$	$V_{\mathrm{T}}^{a}$ (V)	
<b>4</b> a	0.0009	10 <sup>2</sup>	-10	0.0009	10 <sup>2</sup>	-10	0.0009	102	-10	
4b	0.016	$10^2 \sim 10^3$	-5 ~ -4	0.020	$10^2 \sim 10^3$	-5 ~ -8	0.015	$10^2 \sim$	3 ~ 13	
	(0.019)			(0.022)			(0.018)	10 <sup>3</sup>		
4c	0.003	10 <sup>2</sup>	-6 ~ -4	0.003	$10^2 \sim 10^3$	-2 ~ -7	0.003	10 <sup>2</sup>	-2 ~	
	(0.003)			(0.005)			(0.003)	~103	-1	

<sup>a</sup> Typical device characteristics obtained from about 10 devices, and all devices were measured in nitrogen.

**Table S2**. Average (Maximum) mobilities ( $\mu$ ), current on/off ratios ( $I_{on}/I_{off}$ ), and threshold voltages ( $V_T$ ) for thin film of **4a–c** fabricated by spin coating on OTS-treated Si/SiO<sub>2</sub> substrates at different annealing temperatures.

	annealed at 80 °C			annealed at 120 °C			annealed at 160 °C		
	$\mu_{e}^{a} (cm^{2} V^{-1} s^{-1})$	$I_{\rm on}/I_{\rm off}{}^{\rm a}$	$V_{\mathrm{T}}{}^{a}\left(\mathrm{V} ight)$	$\mu_e^a$ (cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup> )	$I_{\rm on}/I_{\rm off}{}^{\rm a}$	$V_{T}^{a}(V)$	$\frac{\mu_{\rm e}^a}{(\rm cm^2 V^{-1} s^{-1})}$	$I_{\rm on}/I_{\rm off}{}^{\rm a}$	$V_{\mathrm{T}}^{a}$ (V)
<b>4</b> a	0.002	10 <sup>2</sup> ~	12 ~ 15	0.003	10 <sup>3</sup> ~	1~4	0.002	$10^2 \sim 10^3$	0 ~ 3
	0.016	$10^{4}$ $10^{3} \sim$	3 ~ 8	0.015	104	2 ~ 5	0.011	10 <sup>3</sup> ~10 <sup>4</sup>	0~4
4b	(0.019)	$10^{4}$		(0.022)	$10^{-5} \sim 10^{-4}$		(0.014)		
4c	0.003	10 <sup>2</sup> ~	22 10	0.003		16 ~ 12	0.003		0 12
	(0.003)	10 <sup>3</sup>	25~18	(0.005)	10 <sup>2</sup>		(0.003)	$10^2 \sim$	9~12
	0.002	$10^3 \sim$	-56 ~	0.002	~10 <sup>3b</sup>	-70 ~	0.0004	10 <sup>3b</sup>	-60 ~
	(0.002) <sup>b</sup>	10 <sup>4b</sup>	-53 <sup>b</sup>	(0.003) <sup>b</sup>		-65 <sup>b</sup>	(0.0008) <sup>b</sup>		-53 <sup>b</sup>

<sup>a</sup> Typical device characteristics obtained from about 10 devices, and all devices were measured in air. <sup>b</sup> hole mobilities.



Figure S7. Comparison of transfer characteristics measured under ambient conditions and N<sub>2</sub> with  $V_{\rm T}$  of 100V (blue: measured in Air; red: measured in N<sub>2</sub>; a, 4a; b, 4b; c, 4c; d, 4c).



9. XRD measurements of thin films of 4a-c.

Figure S8. XRD patterns of spin-coated thin films of 4a–c annealed at 120 °C





#### National Center for Organic Mass Spectrometry in Shanghai Shanghai Institute of Organic Chemistry Chinese Academic of Sciences High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : M162395

Sample Serial Number: WWT-1-1-1

Operator : HUAQIN Date: 2016/09/08

#### Operation Mode: MALDI\_DHB

Elemental composition search on mass 1243.59

m/z=. 1238.	59-1248.59			
m/z	Theo. Mass	Delta	RDB	Composition
		(ppm)	equiv.	
1243.5863	1243.5805	4.65	20.5	C 68 H 100 O 4 N 4 Br S 4



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星期一 9月 26 17:29:26 2016 (GMT+08:00)



## The MS, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and IR spectra of compound 3a



#### National Center for Organic Mass Spectrometry in Shanghai Shanghai Institute of Organic Chemistry Chinese Academic of Sciences High Resolution MS DATA REPORT



Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : M163026

Sample Serial Number: WWT-3-23

Operator :HUAQIN Date: 2016/11/25

#### Operation Mode: DART Positive

Elemental composition search on mass 1309.69

m/z = 1304.	69-1314.69			
m/z	Theo. Mass	Delta	RDB	Composition
		(ppm)	equiv.	
1309.6876	1309.6876	0.02	28.5	C 78 H 103 O 3 N 4 F 2 S 4
	1309.6867	0.70	29.0	C 80 H 102 O 5 N F 3 S 3
	1309.6887	-0.85	24.5	C 75 H 104 O 4 N 4 F 3 S 4
	1309.6889	-1.00	28.0	C 80 H 105 O 4 N F 2 S 4
	1309.6894	-1.36	34.0	C 80 H 97 O 5 N 5 F 2 S 2
	1309.6853	1.73	29.5	C 78 H 100 O 4 N 4 F 3 S 3
	1309.6900	-1.87	24.0	C77 H106 O5 N F3 S4
	1309.6914	-2.90	29.0	C 78 H 102 O N 5 F 3 S 4
	1309.6837	2.94	28.0	C 78 H 104 O 5 N 3 F S 4
	1309.6916	-3.06	33.0	C 80 H 100 O 4 N 5 F S 3







The MS, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and IR spectra of compound 3b



National Center for Organic Mass Spectrometry in Shanghai Shanghai Institute of Organic Chemistry Chinese Academic of Sciences High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card, Serial Number : M162399

Sample Serial Number: wwt-3-22

Operator : HUAQIN Date: 2016/09/08

#### Operation Mode: MALDI\_DHB

Elemental composition search on mass 1241.70

m/z= 1236.70-1246.70

m/z	Theo.	Mass	Delta	RDB	Composition
			(ppm)	equiv.	
1241.6994	1241.	6993	0.08	29.0	C 79 H 103 O 5 N S 3
	1241.	7006	-1.00	34.0	C 80 H 99 O N 5 S 3
	1241.	6979	1.16	29.5	C77 H101 O4 N4 S3
	1241.	7013	-1.55	24.5	C74 H105 O4 N4 S4
	1241.	7027	-2.63	24.0	C76 H107 O5 N S4
	1241.	7040	-3.71	29.0	C 77 H 103 O N 5 S 4
	1241.	6946	3.88	34.5	C 80 H 97 O 4 N 4 S 2
	1241.	6941	4.26	28.5	C 80 H 105 O 3 S 4
	1241.	7053	-4.79	28.5	C 79 H 105 O 2 N 2 S 4



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星期一 9月 26 17:33:43 2016 (GMT+08:00)



The MS, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and IR spectra of compound 3c







# The MS, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, IR spectra and element analysis of compound 4a





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## The MS, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, IR spectra and element analysis of

#### compound 4b







## The MS, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, IR spectra and element analysis of

#### compound 4c







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