

Electronic Supporting Information for:

Larger π -Extended *anti*-/*syn*-Aroylenediimidazole Polyaromatic Compounds: Synthesis, Physical Properties, Self-Assembly, and Quasi-linear Conjugation Effect

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Monoisotopic Mass, Even Electron Ions
 7 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 55-60 H: 40-45 N: 5-8 O: 0-7
 C₅₈H₄₄N₆O₆
 LIULE11 3 (0.082)

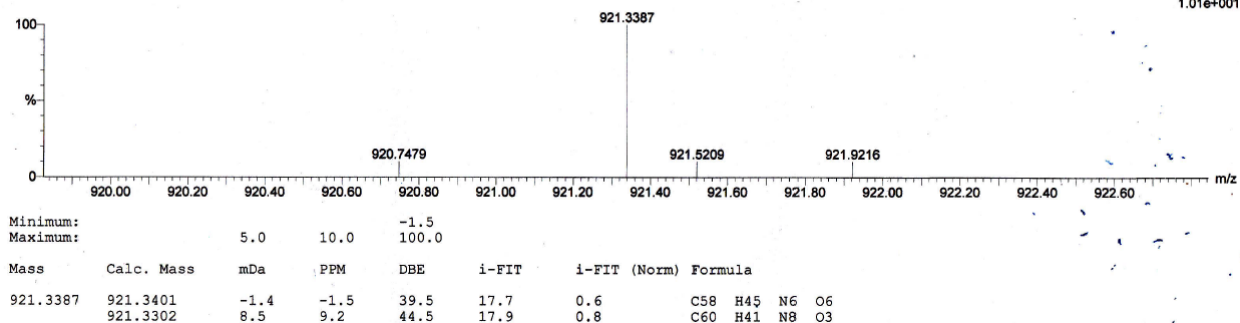
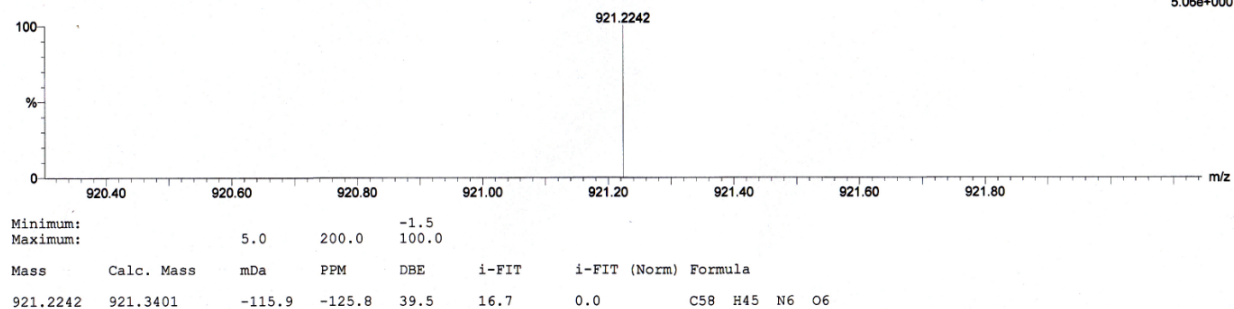


Figure S1. HiRes MALDI-TOF MS of A1

Monoisotopic Mass, Even Electron Ions
 1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 57-58 H: 44-45 N: 5-6 O: 5-6
 C₁₃₃H₄₂N₃O₃₀Br
 ZHC-19 3 (0.083)

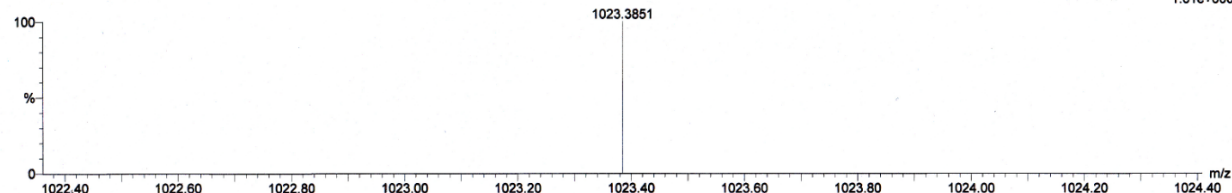


5 Figure S2. HiRes MALDI-TOF MS of A2

Monoisotopic Mass, Even Electron Ions
 18 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 63-65 H: 45-48 N: 7-9 O: 5-7 Br: 0-2

C133H42N32O30Br
 ZHC-9 10 (0.242)

1: TOF MS ES+
 1.01e+000



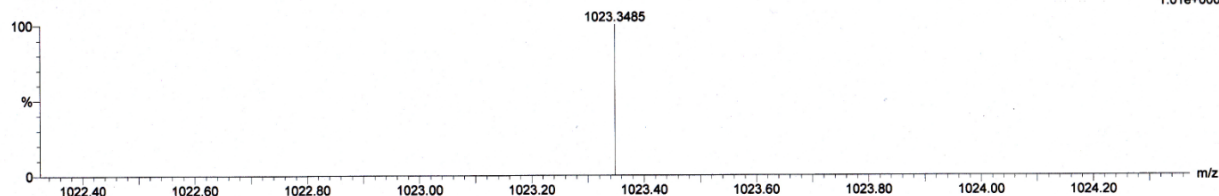
Minimum:				-1.5				
Maximum:		5.0	200.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula	
1023.3851	1023.3619	23.2	22.7	45.5	11.1	0.0	C64	H47 N8 O6

Figure S3. HiRes MALDI-TOF MS of **B1**

Monoisotopic Mass, Even Electron Ions
 18 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 63-65 H: 45-48 N: 7-9 O: 5-7 Br: 0-2

C133H42N32O30Br
 ZHC-8 1 (0.045)

1: TOF MS ES+
 1.01e+000



Minimum:				-1.5				
Maximum:		5.0	20.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula	
1023.3485	1023.3619	-13.4	-13.1	45.5	12.7	0.0	C64	H47 N8 O6

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Figure S4. HiRes MALDI-TOF MS of **B2**

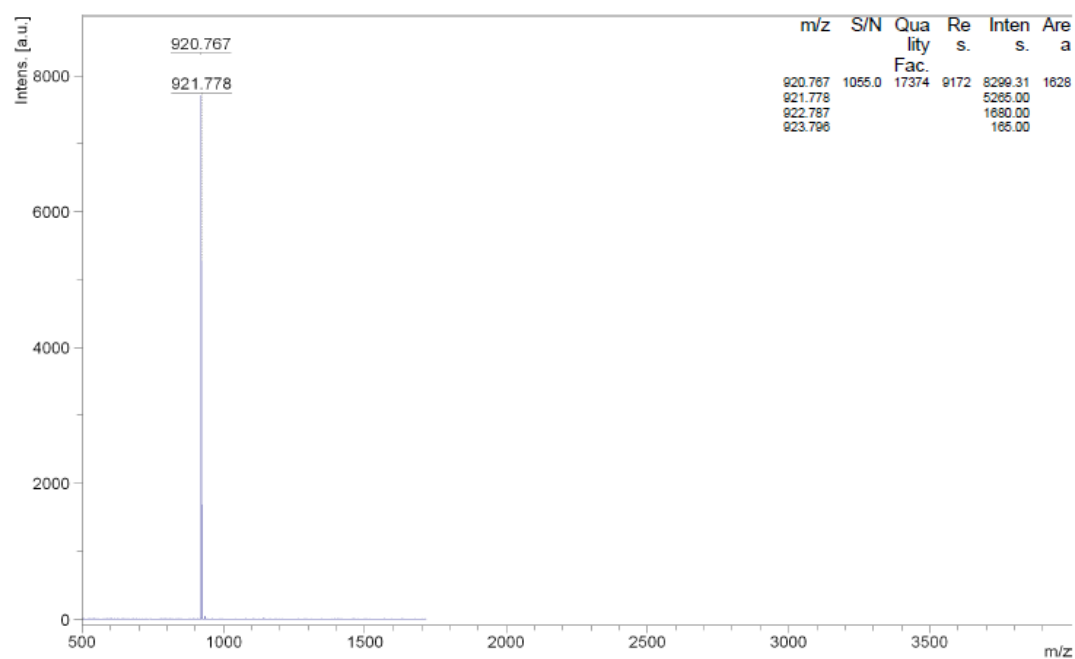


Figure S5. MALDI-TOF MS of A1

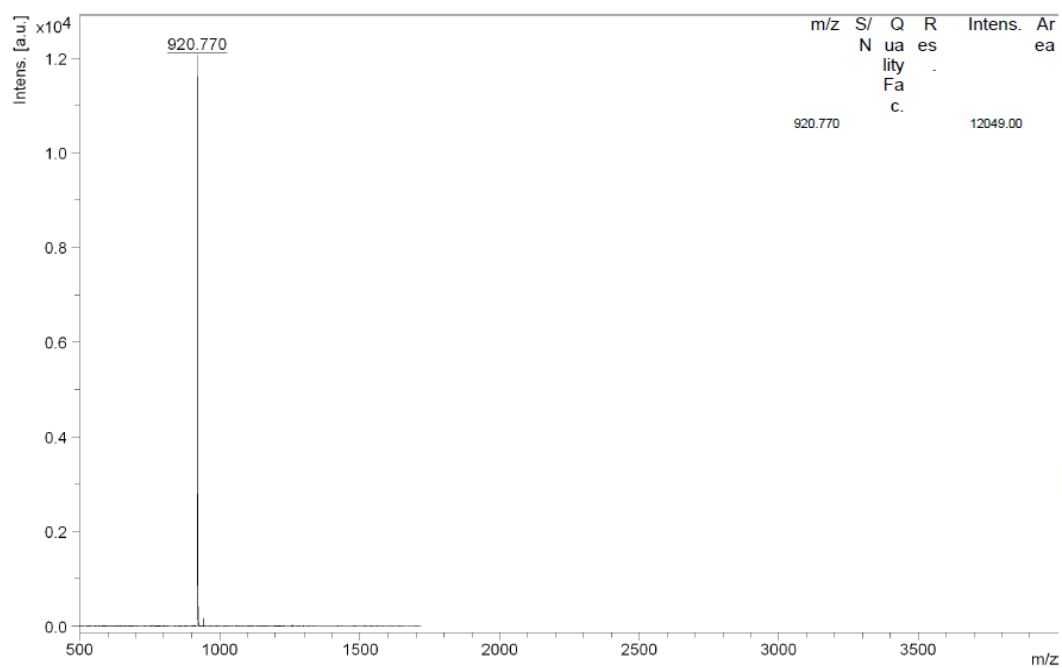


Figure S6. MALDI-TOF MS of A2

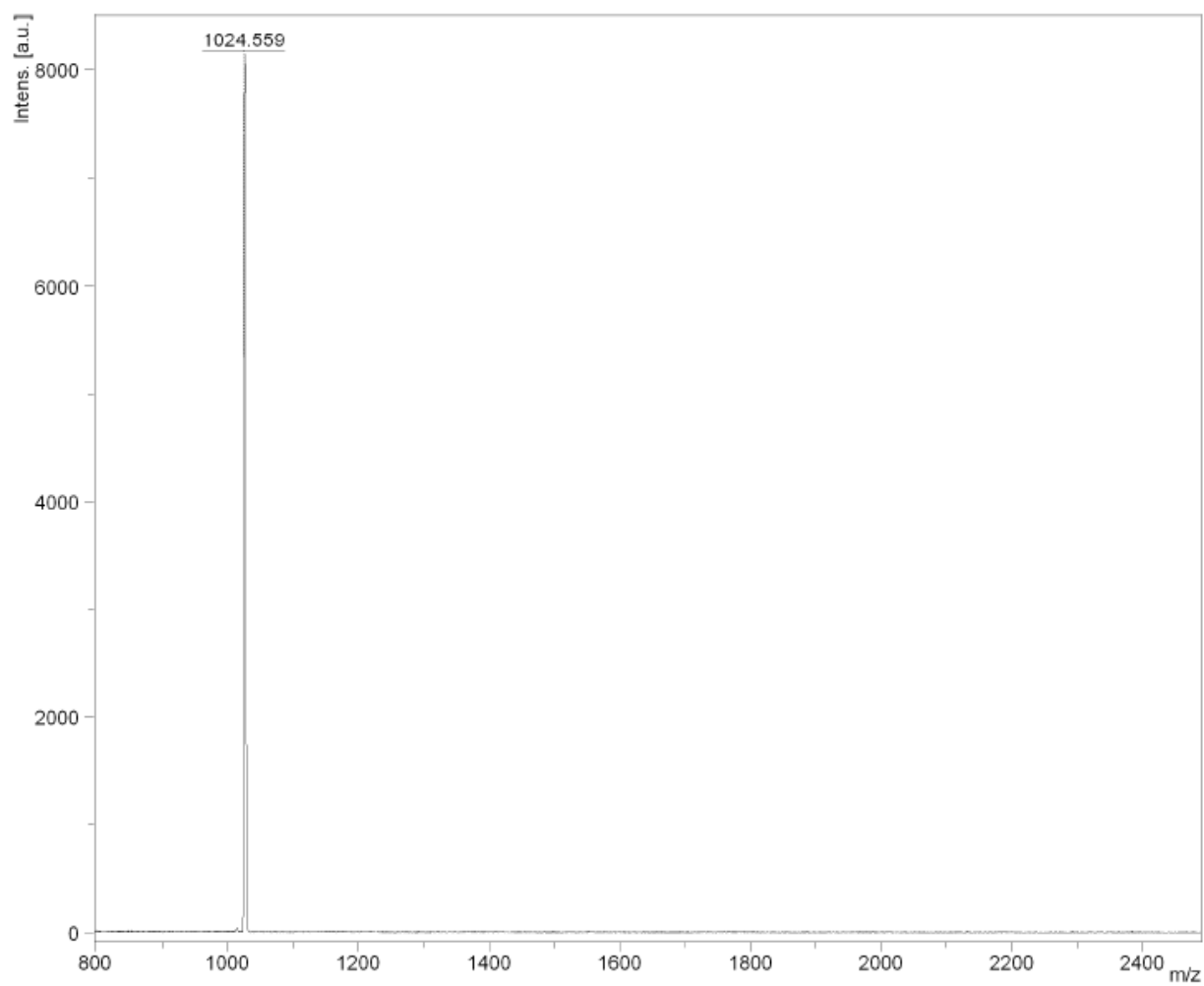


Figure S7. MALDI-TOF MS of **B1**

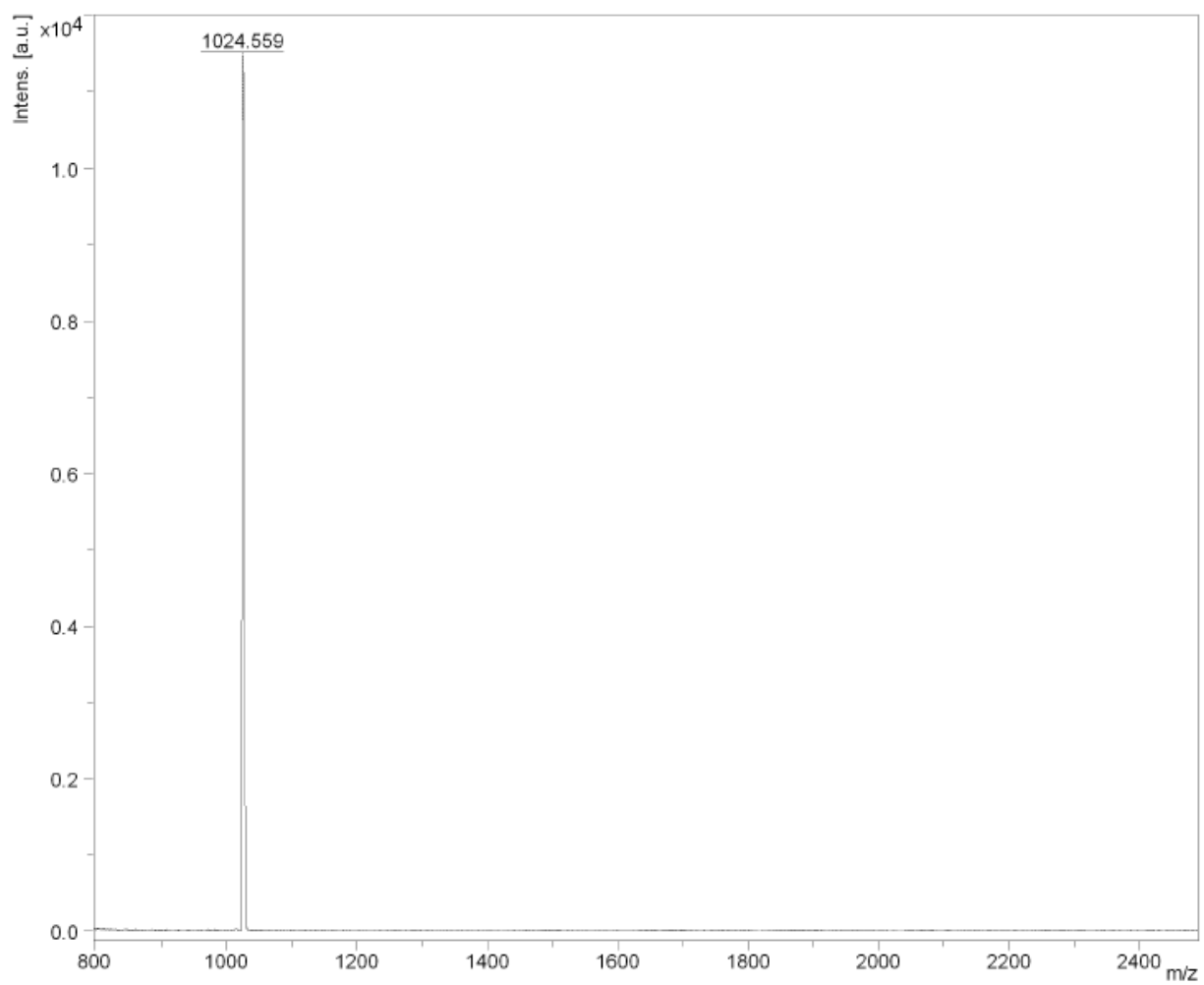
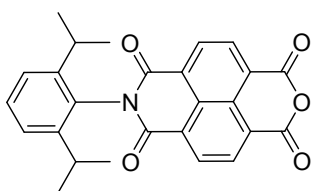


Figure S8. MALDI-TOF MS of **B2**



NIA

Chemical Formula: $C_{26}H_{21}NO_5$

Exact Mass: 427.14

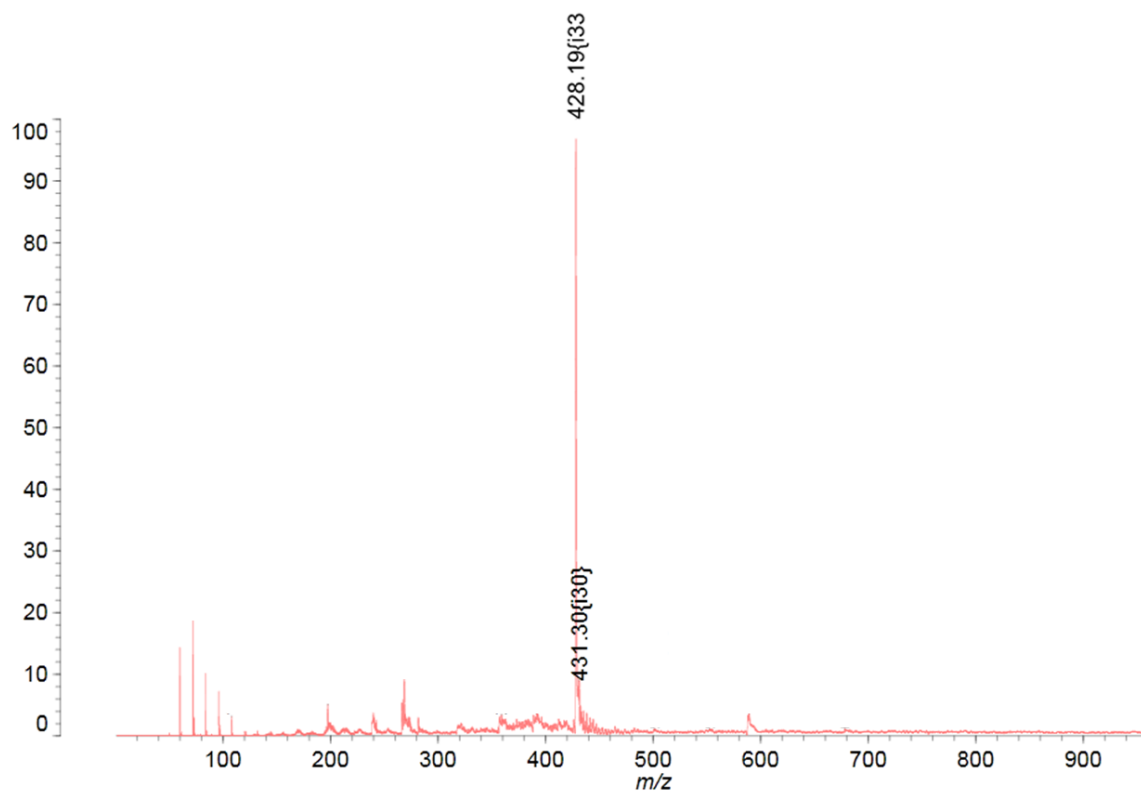


Figure S9 MALDI TOF MS of **NIA** without further purification¹

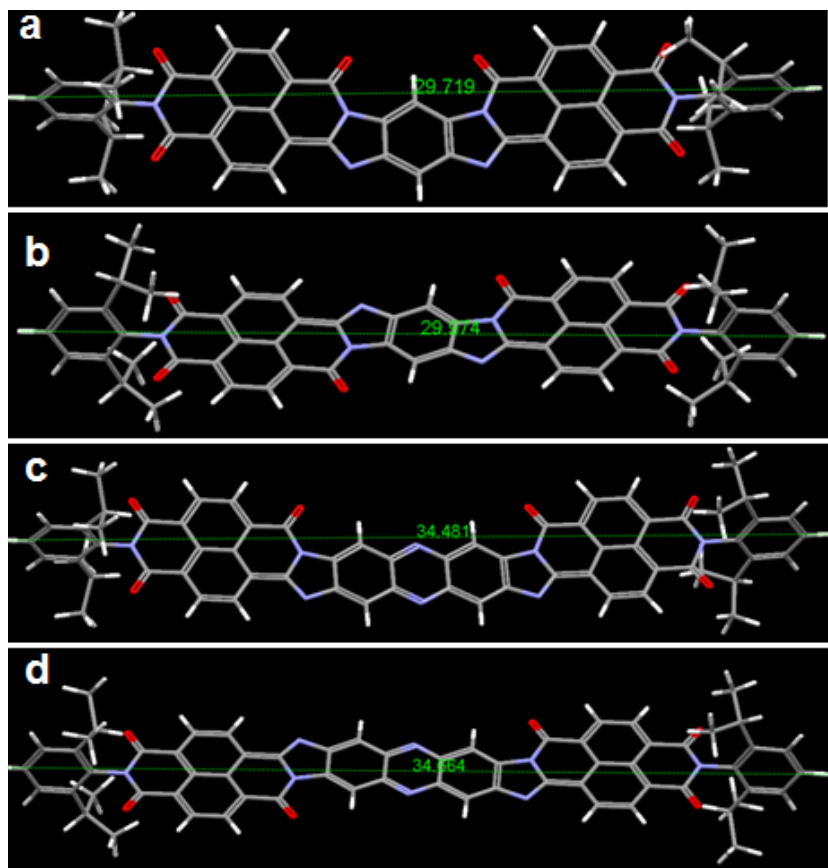


Figure S10 The whole molecular length (2.97, 3.00, 3.45, and 3.47 nm) of **A1**, **A2**, **B1**, and **B2**, respectively.

5 Reference:

Zhao, J.; Li, G.; Wang, C.; Chen, W.; Loo, J.; Zhang, Q. *RSC Adv.* **2013**, 3, 9653-9657.