

Supporting Information
of
Synthesis and Aggregation Behavior of Poly(arylene alkenylene)s
and Poly(arylene alkylene)s Having Dialkoxyphenylene and
Aromatic Diimide Groups

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Figure S1.	¹ H NMR spectra (a) of poly(1a-IA) before Soxhlet extraction (b) of a soluble fraction of the polymer obtained by Soxhlet extraction for 20 h using THF as the solvent	1
Figure S2.	¹ H NMR spectrum of poly(1b-IA)	2
Figure S3.	¹³ C{ ¹ H} NMR spectrum of poly(1b-IA)	2
Figure S4.	¹ H NMR spectrum of poly(1a-IIA)	3
Figure S5.	¹ H NMR spectrum of poly(1c-IA)	3
Figure S6.	¹ H NMR spectrum of poly(1b-IA-H)	4
Figure S7.	¹³ C{ ¹ H} NMR spectrum of poly(1b-IA-H)	4
Figure S8.	¹ H NMR spectrum of poly(1c-IA-H)	5
Figure S9.	¹³ C{ ¹ H} NMR spectrum of poly(1c-IA-H)	5
Figure S10.	¹ H NMR spectrum of poly(1a-IIA-H)	6
Figure S11.	¹³ C{ ¹ H} NMR spectrum of poly(1a-IIA-H)	6
Figure S12.	MALDI-TOF Mass of poly(1a-IA)	7
Figure S13.	MALDI-TOF Mass of poly(1a-IIA)	8
Figure S14.	(a)ESI-MS spectrum of poly(1a-IA). (b) Observed isotope pattern for 1:1 adduct of 1a and IA . (c) Calculated isotope pattern for the cyclic 1:1 adduct.	9
Figure S15.	(a)ESI-MS spectrum of poly(1a-IIA). (b) Observed isotope pattern for 1:1 adduct of 1a and IIA . (c) Calculated isotope pattern for the cyclic 1:1 adduct.	12
Figure S16.	Results of light scattering measurement for poly(1a-IC).	14
Figure S17.	WXR for poly(1a-IC)	15

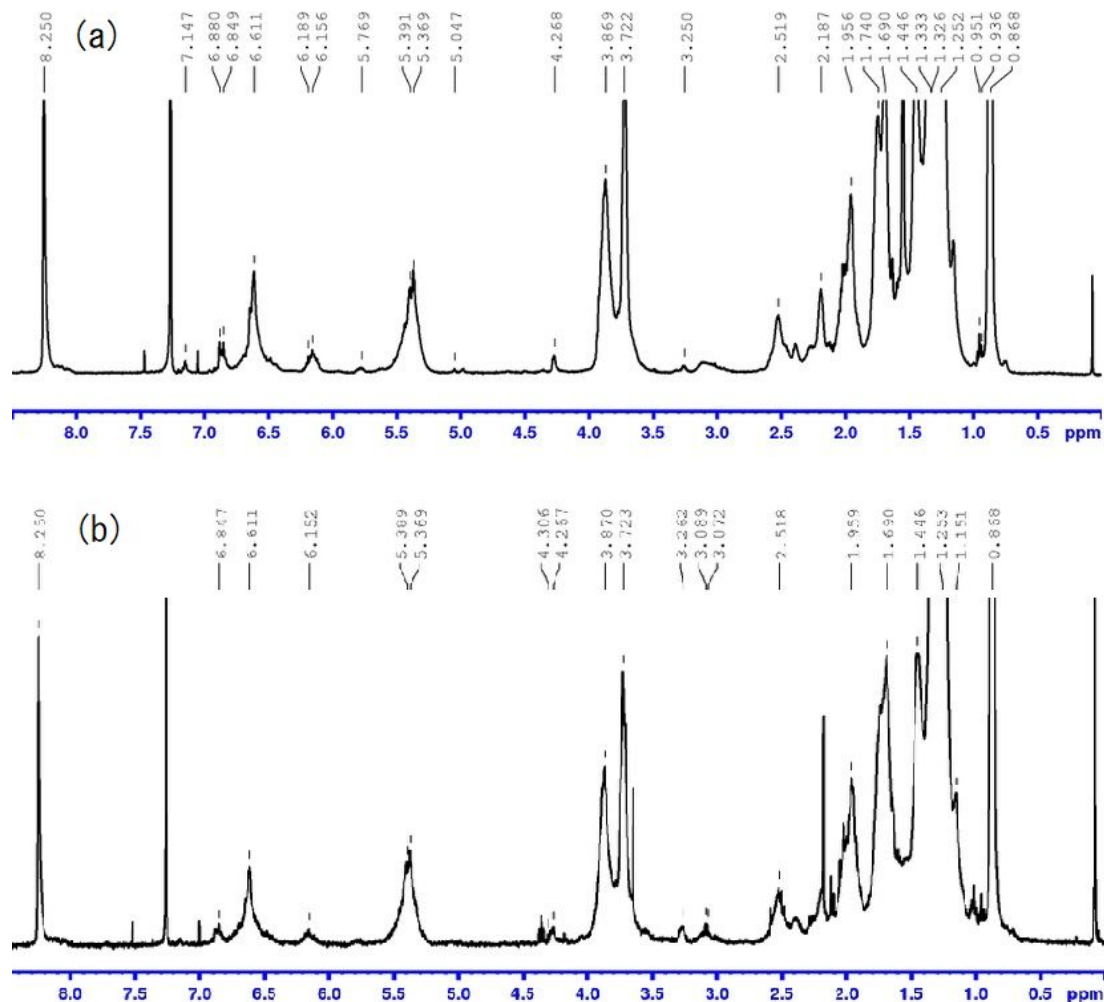


Figure S1. ¹H NMR spectra of poly(1a-IA) (a) before Soxhlet extraction ($M_n = 7600$, PDI = 4.6) (500 MHz, $CDCl_3$, r.t), (b) of soluble fraction obtained by Soxhlet extraction for 20 h using THF as the solvent ($M_n = 5100$, PDI = 2.7) (500 MHz, $CDCl_3$, r.t).

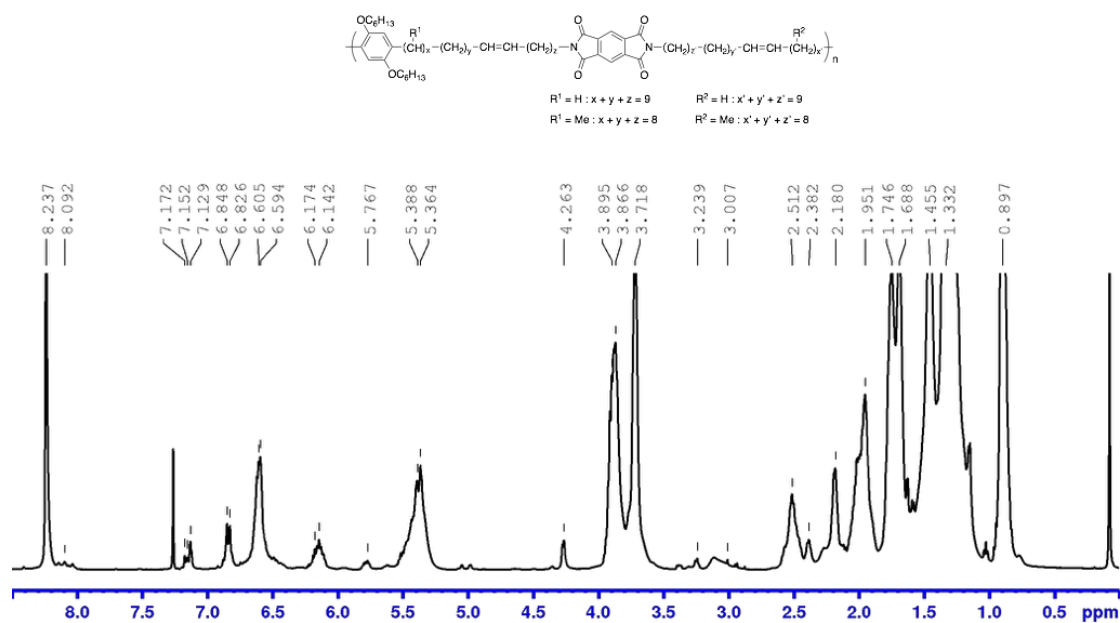


Figure S2. ^1H NMR spectrum of poly(**1b-IA**) (500 MHz, CDCl_3 , r.t.).

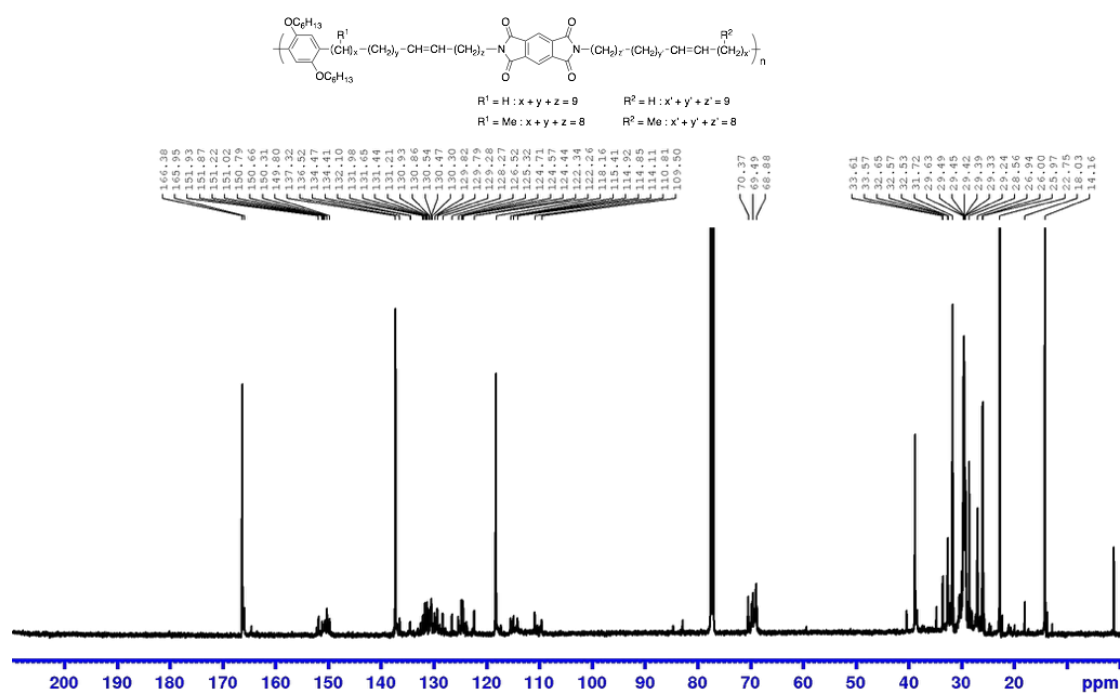


Figure S3. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of poly(**1b-IA**) (125 MHz, CDCl_3 , r.t.).

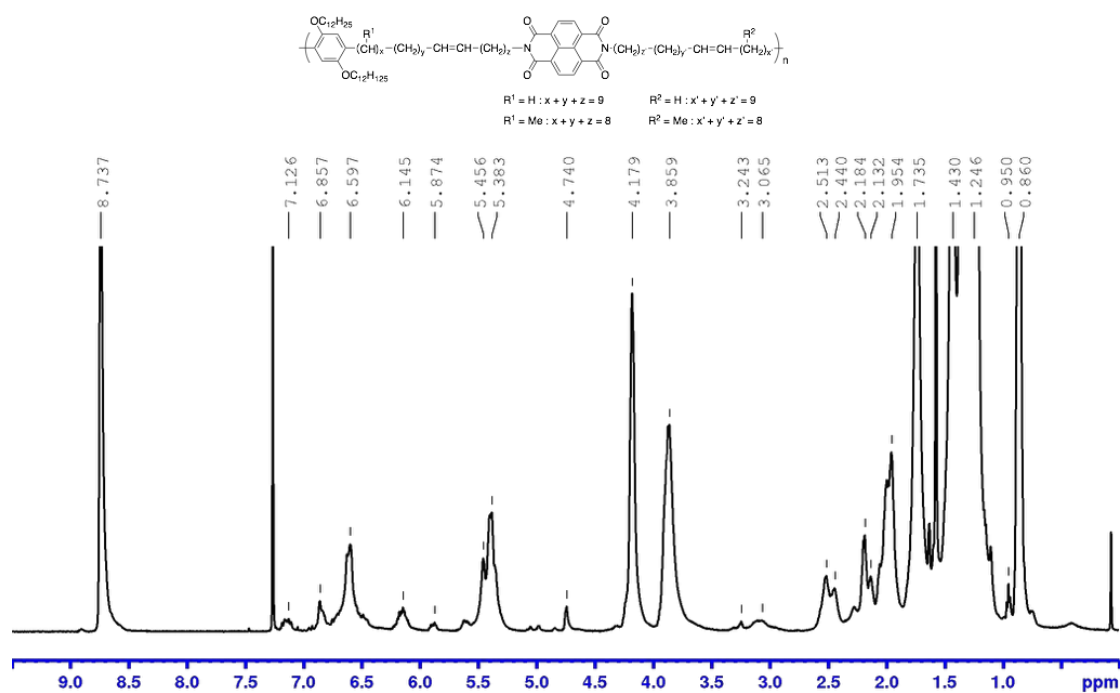


Figure S4. 1H NMR spectrum of poly(1a-IIA) (500 MHz, $CDCl_3$, r.t.).

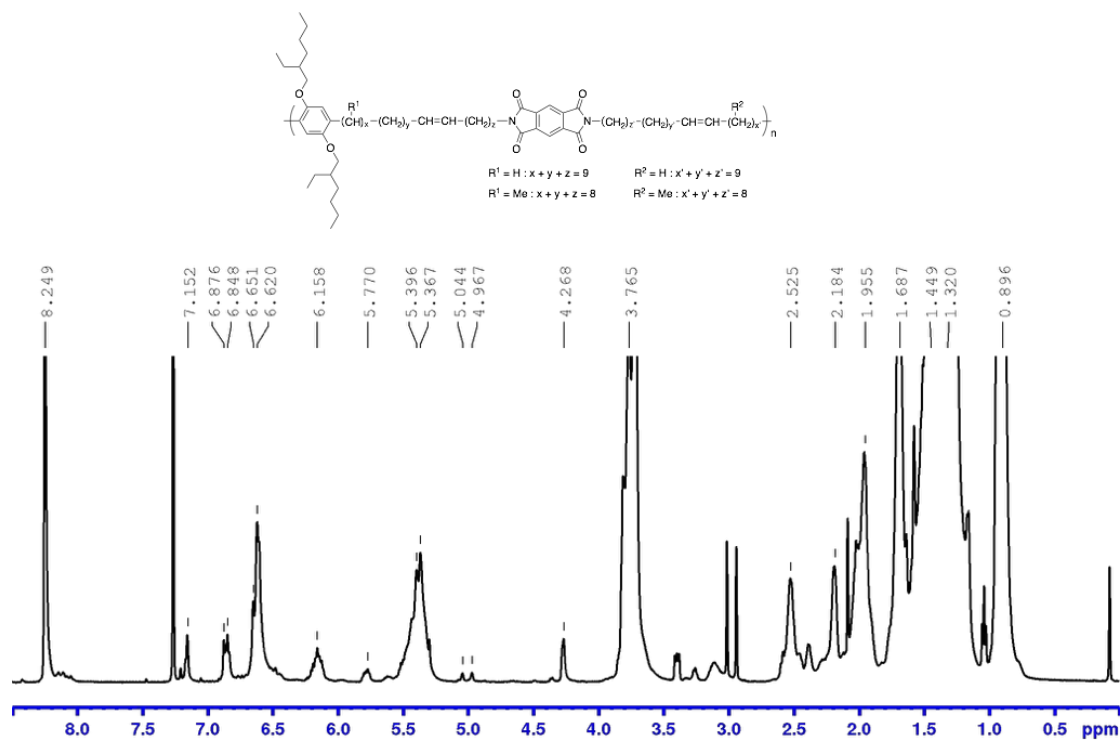


Figure S5. 1H NMR spectrum of poly(1c-IA) (500 MHz, $CDCl_3$, r.t.).

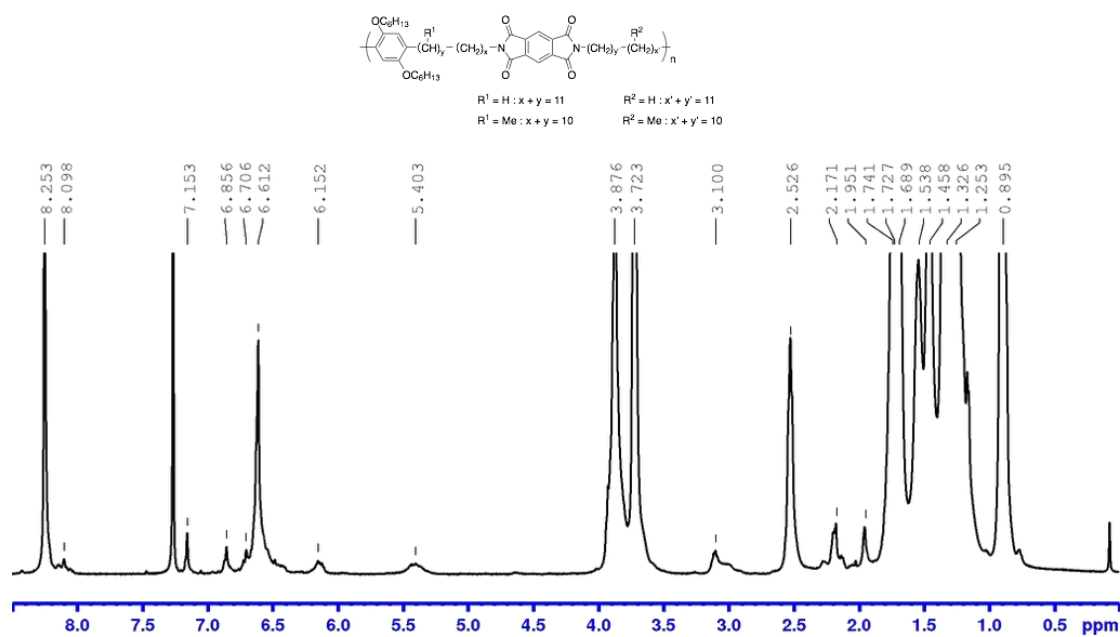


Figure S6. ¹H NMR spectrum of poly(**1b-IA-H**) (500 MHz, CDCl₃, r.t.).

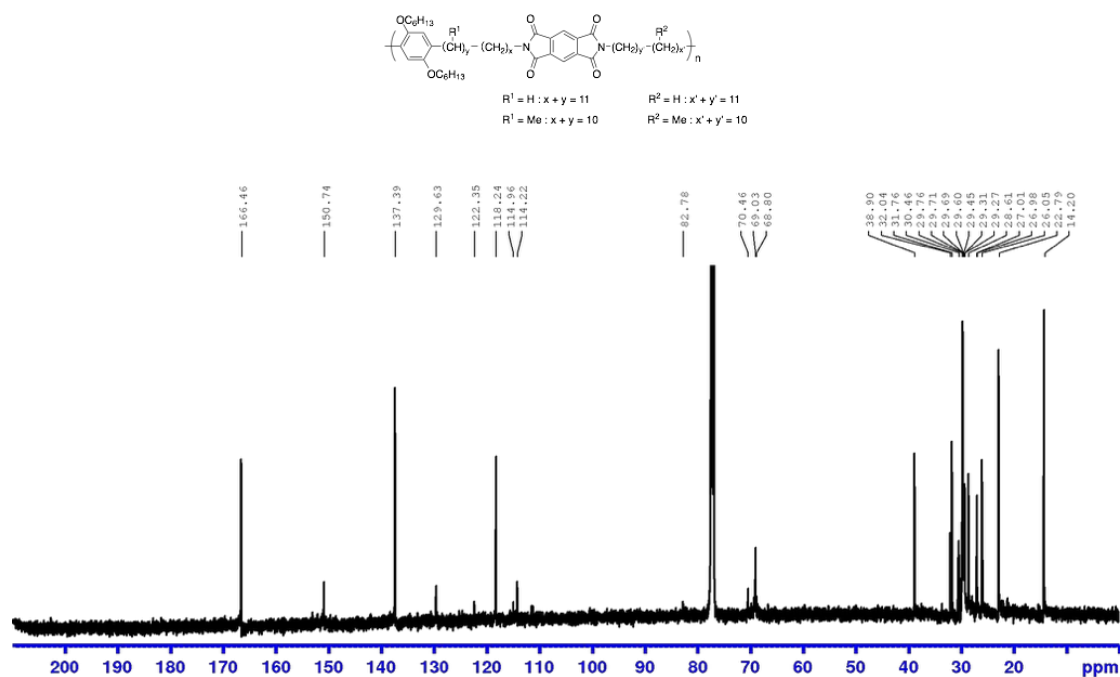


Figure S7. ¹³C{¹H} NMR spectrum of poly(**1b-IA-H**) (125 MHz, CDCl₃, r.t.).

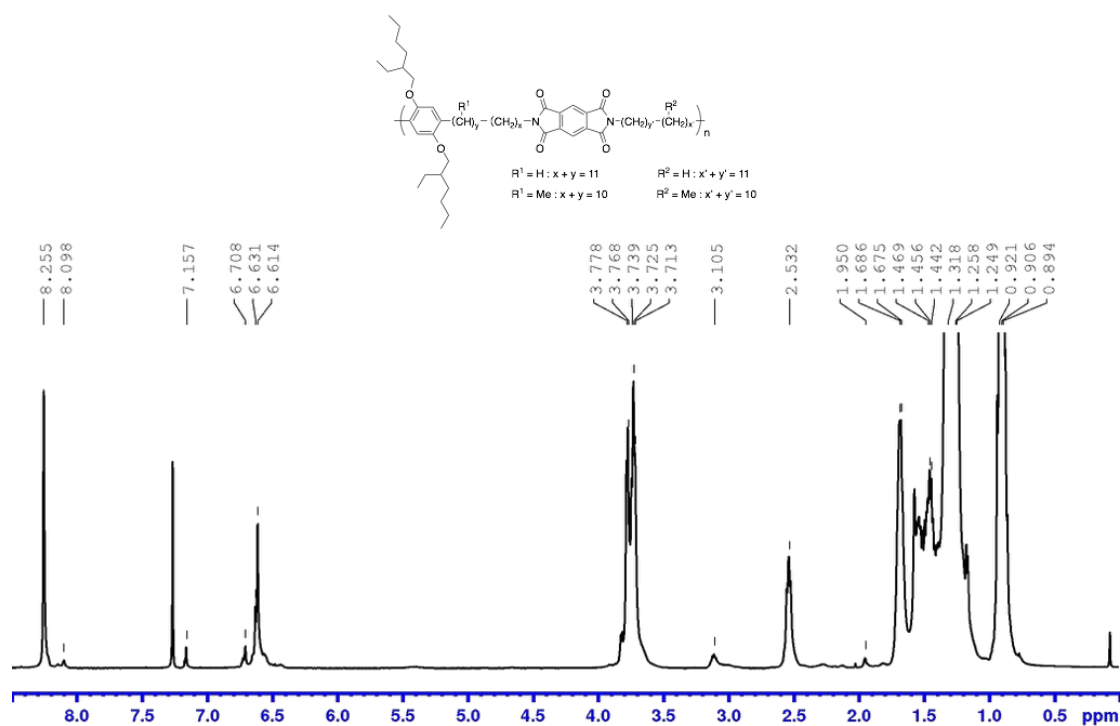


Figure S8. 1H NMR spectrum of poly(1c-IA-H) (500 MHz, $CDCl_3$, r.t.).

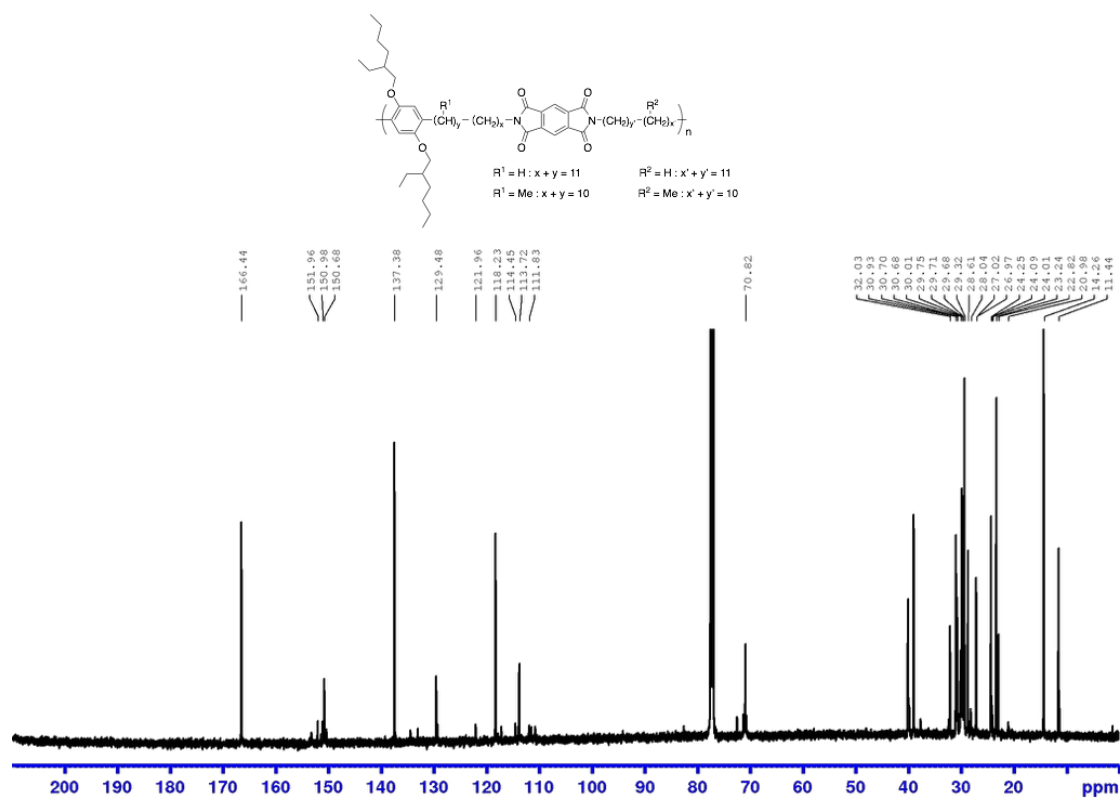


Figure S9. $^{13}C\{^1H\}$ NMR spectrum of poly(1c-IA-H) (125 MHz, $CDCl_3$, r.t.).

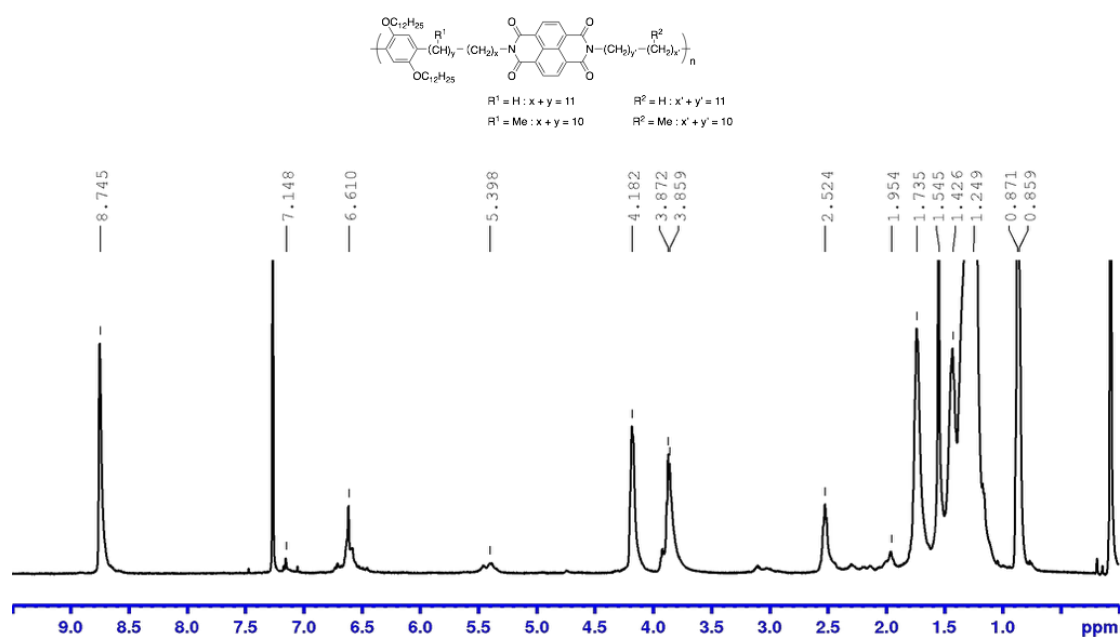


Figure S10. ^1H NMR spectrum of poly(**1a-IIA-H**) (500 MHz, CDCl_3 , r.t.).

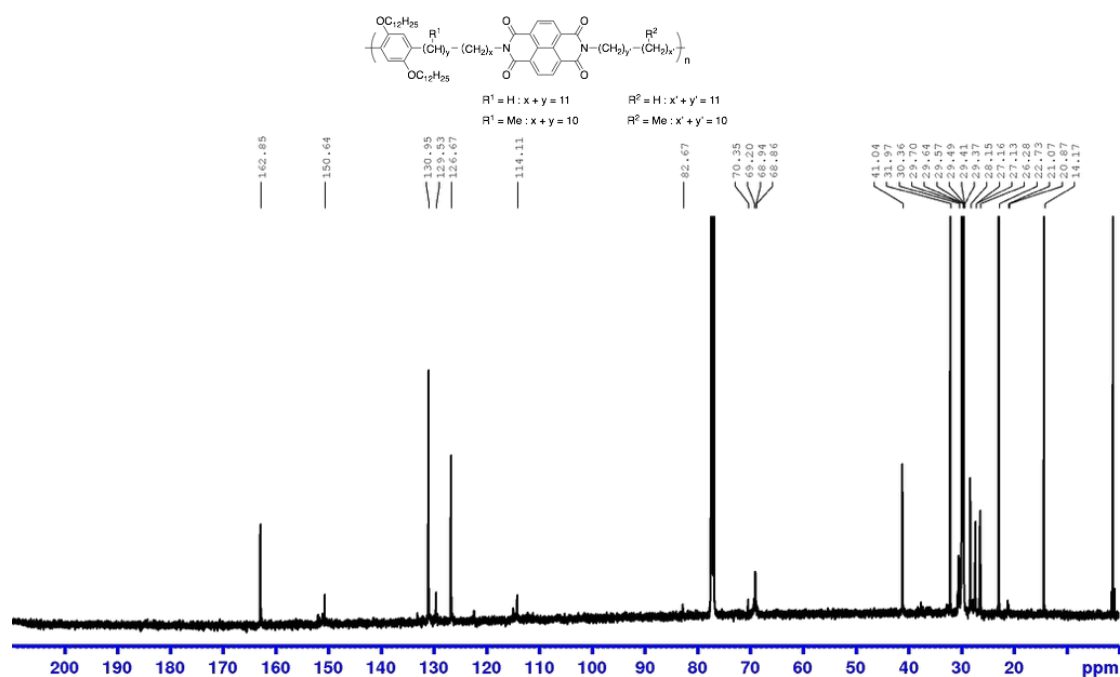


Figure S11. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of poly(**1a-IIA-H**) (125 MHz, CDCl_3 , r.t.).

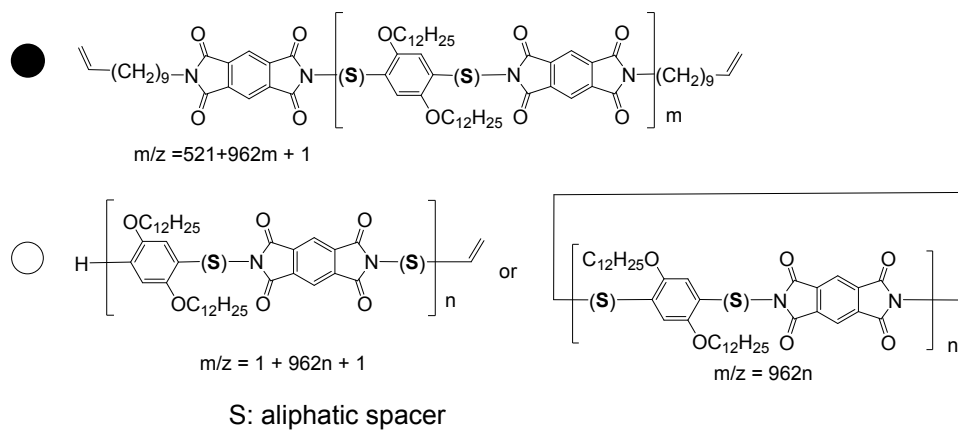
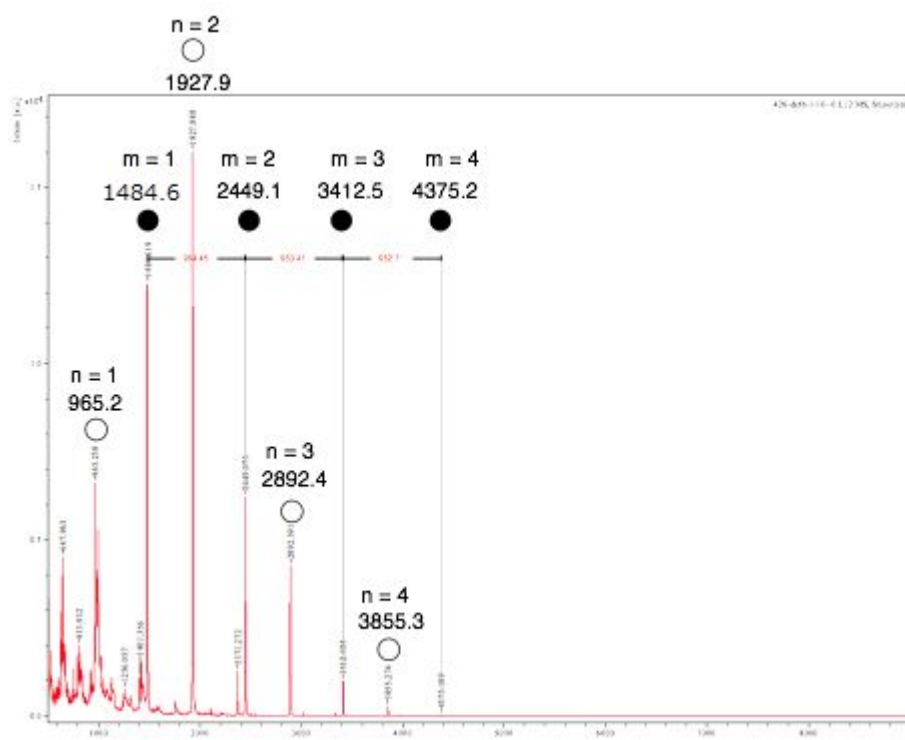


Figure S12. MALDI-TOF Mass of poly(**1a-1A**) (10 mg/mL polymer samples in THF solution with 10 mg/mL DCTB as matrix). Contents of the cyclic oligomers were not determined because of the absence for the information of the isotope pattern.

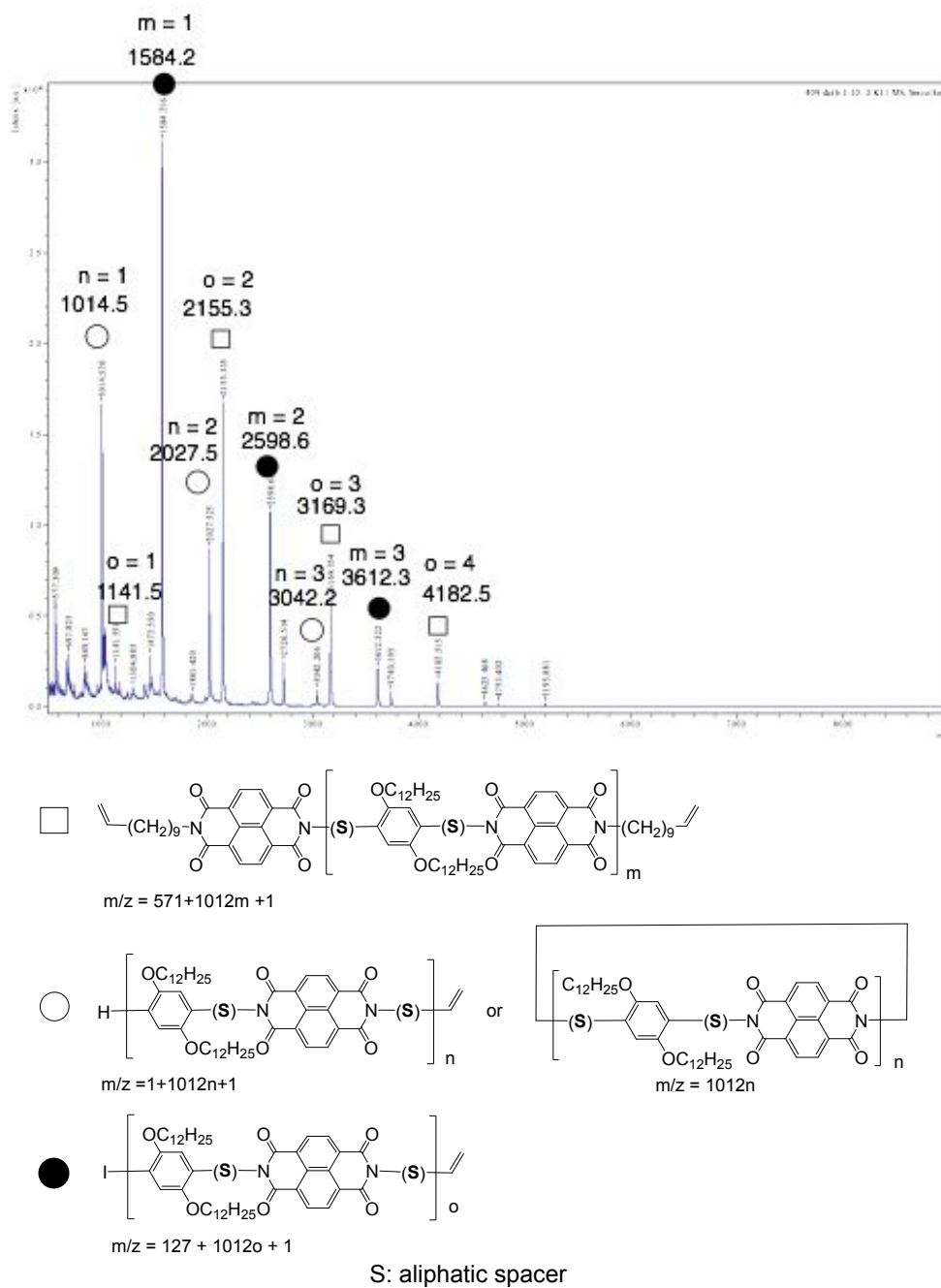
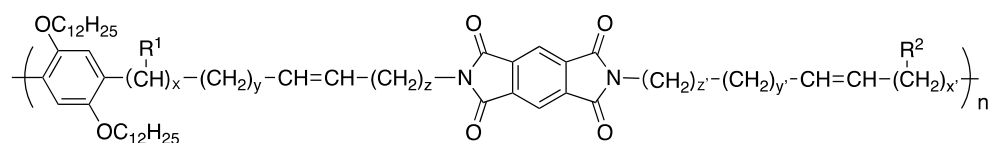


Figure S13. MALDI-TOF Mass of poly(**1a-IIA**) (10 mg/mL polymer samples in THF solution with 10 mg/mL DCTB as matrix). Contents of the cyclic oligomers were not determined because of the absence for the information of the isotope pattern.

ESI-MASS for poly(**1a-IA**)

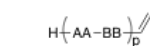
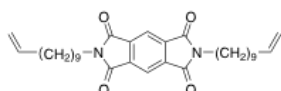
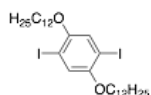


$$\text{R}^1 = \text{H} : x + y + z = 9$$

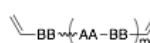
$$\text{R}^2 = \text{H} : x' + y' + z' = 9$$

$$\text{R}^1 = \text{Me} : x + y + z = 8$$

$$\text{R}^2 = \text{Me} : x' + y' + z' = 8$$



$$m/z = 1 + 1 + 962p + 23$$



$$m/z = 520 + 1 + 962m + 23$$



$$m/z = 962n + 23$$



$$m/z = 127 + 1 + 962o + 23$$



Display Report

Analysis Info

Analysis Name D:\Data\osakada\tan\181022\426-000001.d
Method esi_posi_low.m
Sample Name 426-
Comment

Acquisition Date 2018/10/19 10:09:33

Operator BDAL@DE

Instrument micrOTOF 213750.10321

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active			Set Dry Heater	180 °C
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Scan End	2500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

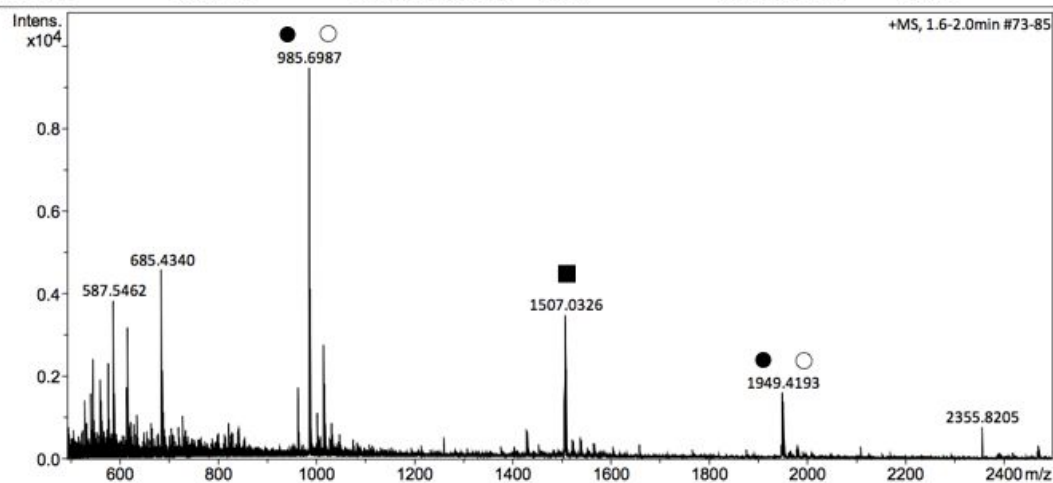


Figure S14. (a)ESI-MS spectrum of poly(**1a-IA**) ($M_n = 7600$, PDI = 4.6 by GPC).

Display Report

Analysis Info

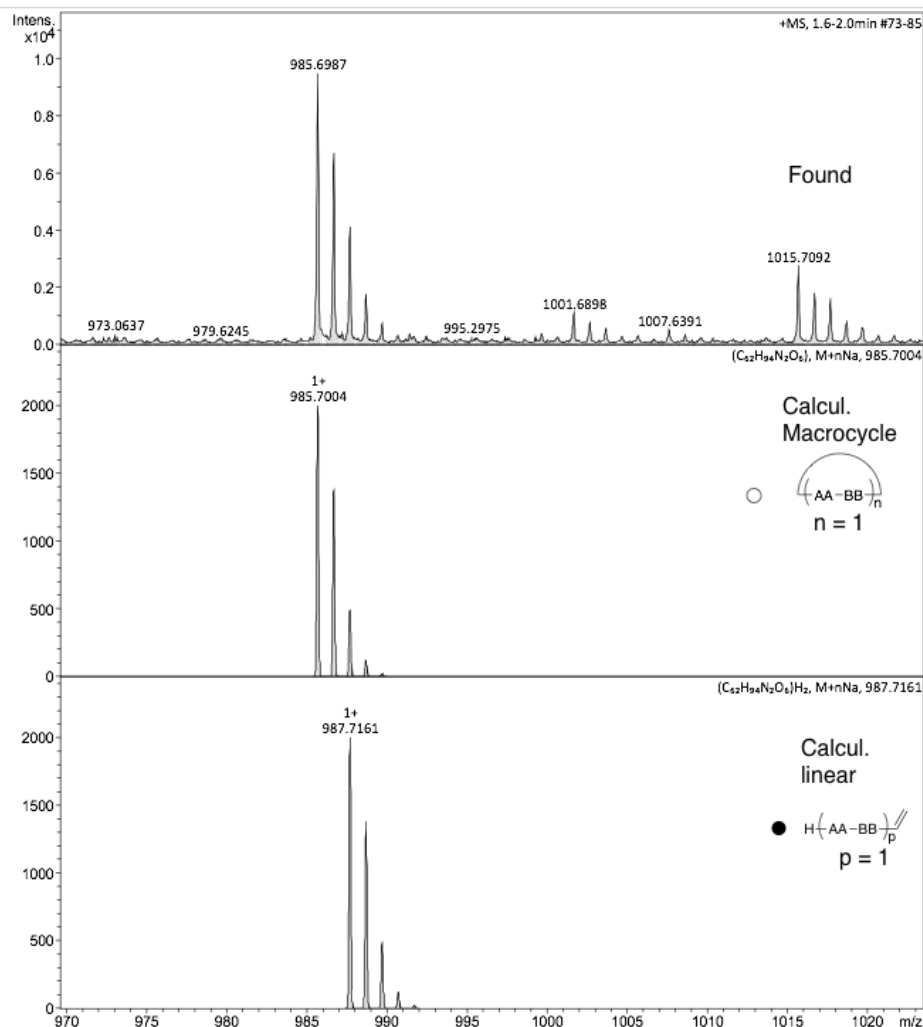
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 Sample Name 426-
 Comment

Acquisition Date 2018/10/19 10:09:33

Operator BDAL@DE
 Instrument micrOTOF 213750.10321

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Bruker Compass DataAnalysis 4.2

printed: 2018/10/22 12:14:35

by: BDAL@DE

1 of 1

Figure S14. (b) Observed and simulated isotope pattern for 1:1 adduct of **1a** and **IA**. Na^+ is derived from the ion source, sodium trifluoroacetate.

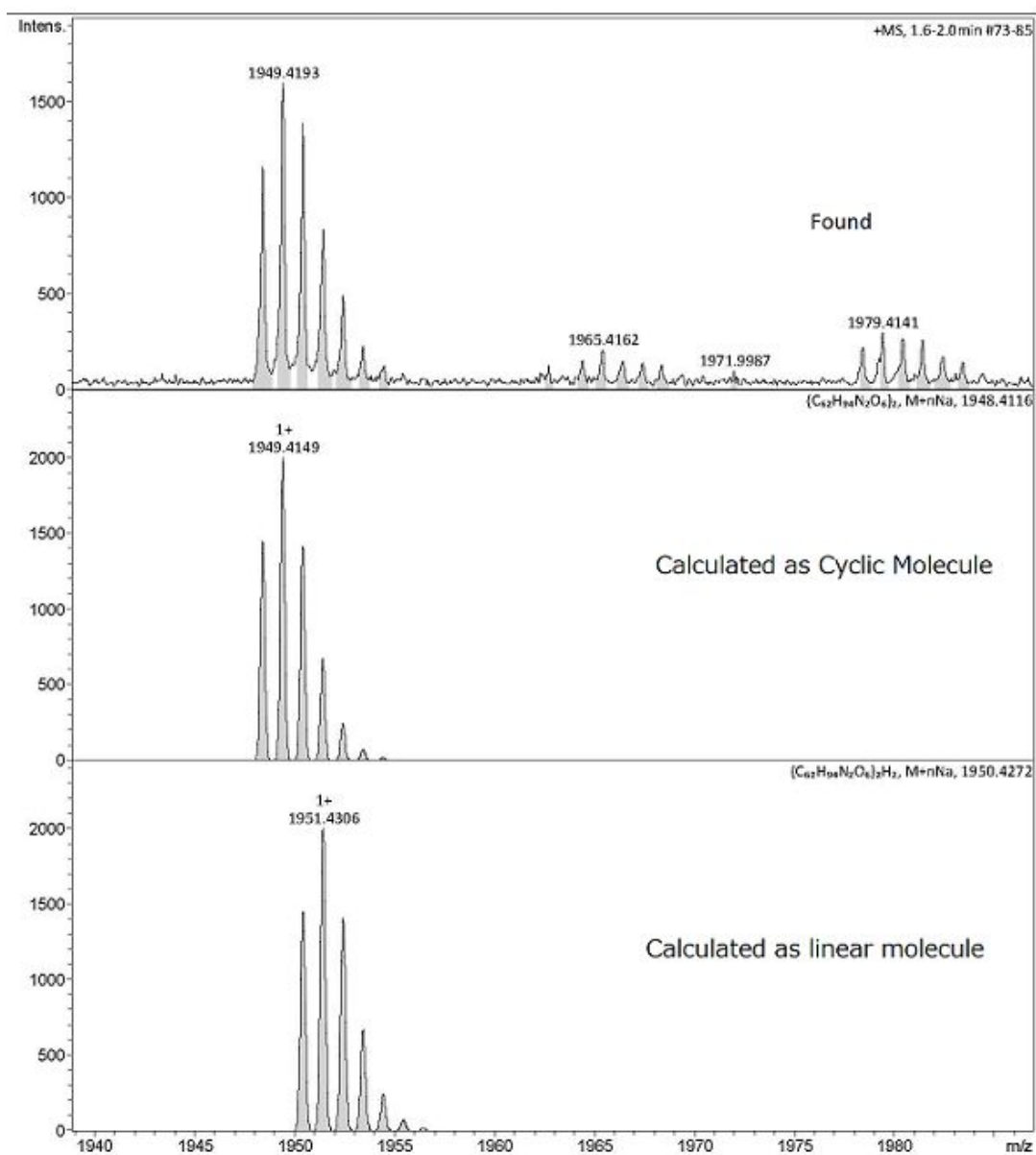
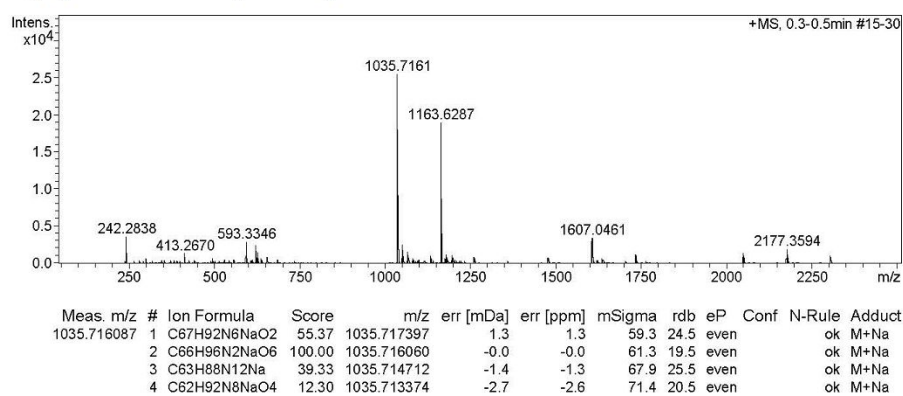


Figure S14. (c) Observed and simulated isotope pattern for 2:2 adduct of **1a** and **IA**.

(a) Observed (total) TDCMAS ESI-TOF



(b) Peaks of 1:1 adduct TDCMAS ESI-TOF

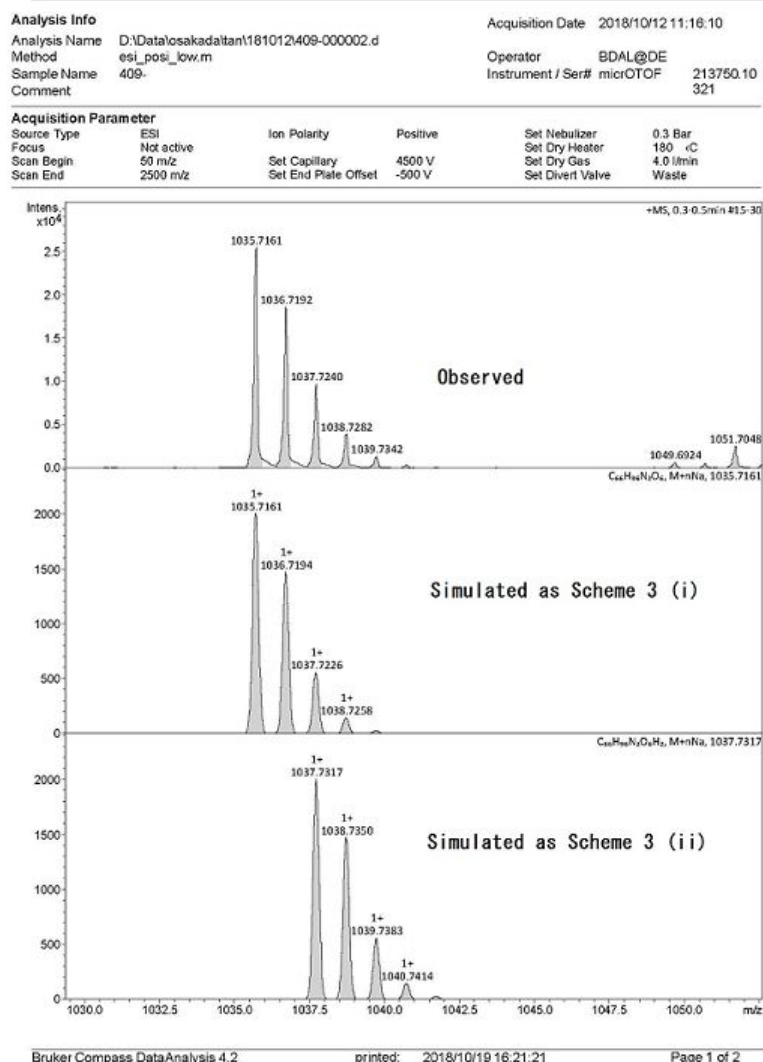


Figure S15. (a) ESI-MS spectrum of poly(**1a-IIA**) ($M_n = 3800$, PDI = 1.7 by GPC). (b) Observed and simulated isotope pattern for 1:1 adduct of **1a** and **IIA**. Na⁺ is derived from the ion source, sodium trifluoroacetate.

(c) Peaks of 2:2 adducts TDCMAS ESI-TOF

Analysis Info		Acquisition Date 2018/10/12 11:16:10	
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Sample Name	409-		321
Comment			

Acquisition Parameter					
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Focus	Not active			Set Dry Heater	180 °C
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Scan End	2500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

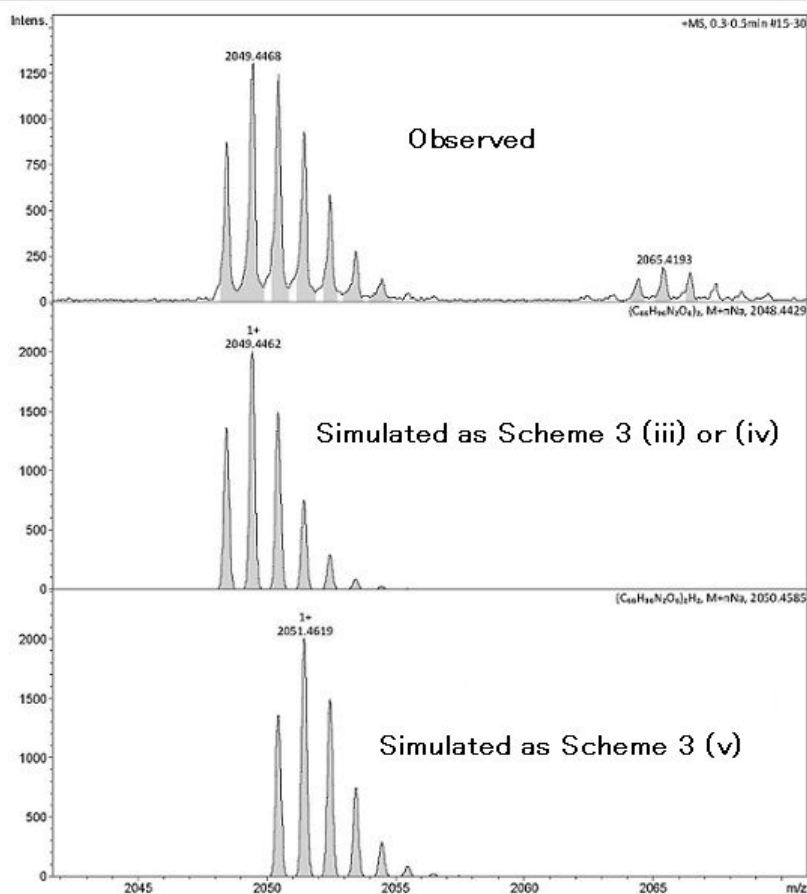
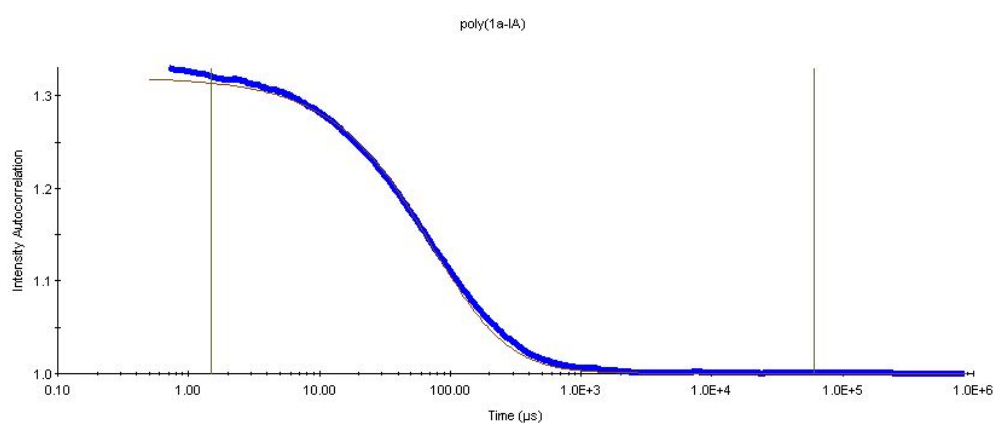
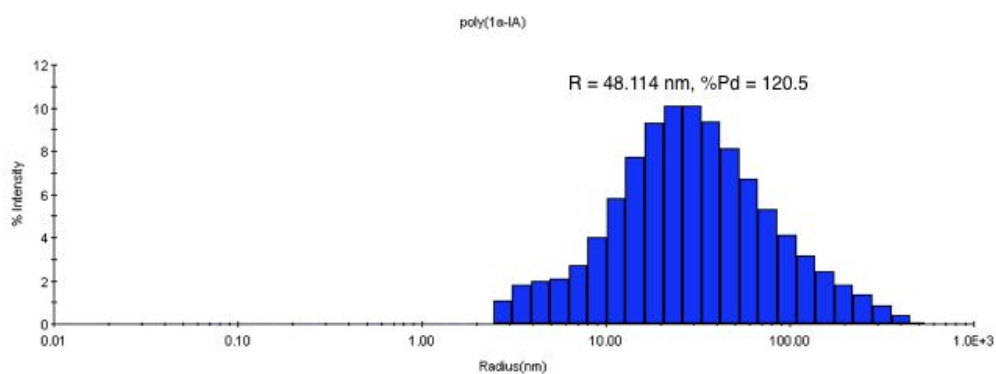


Figure S15. (c) Observed and simulated isotope pattern for 2:2 adduct of **1a** and **IIA**.

Correlation Function



Regularization results



The DynaPro NanoStar of Wyatt Technology Corporation was used for the

Figure S16. Results of light scattering measurement for poly(**1a-IC**).

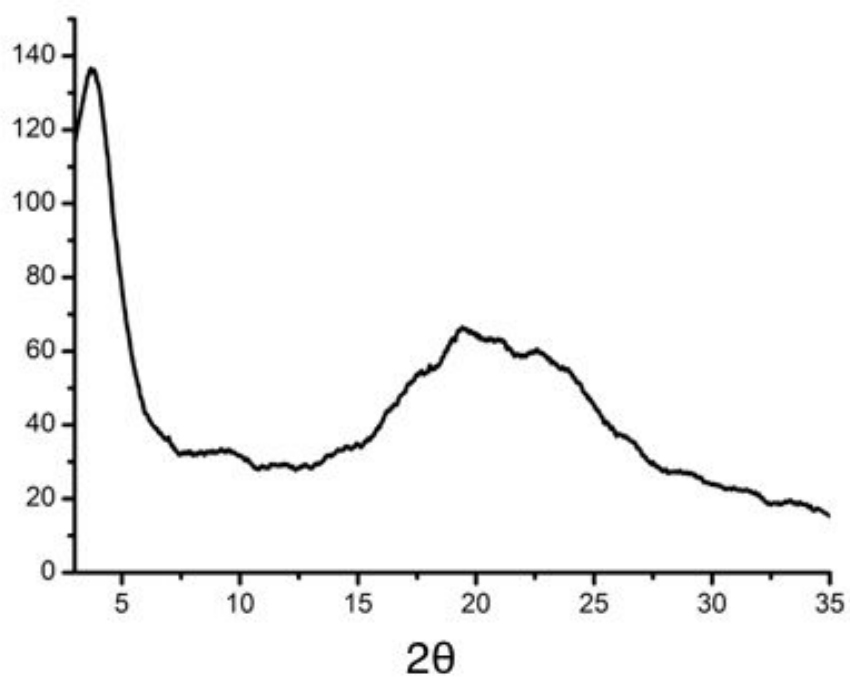


Figure S17. WAXRD for poly(**1a-IC**).