Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

A novel one-pot process for preparation of linear and hyperbranched polycarbonates of various diols and triols using dimethyl carbonate

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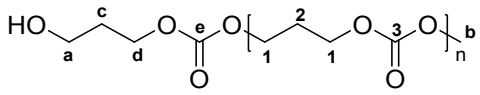
- **^{1}H and ^{13}C NMR spectra of linear and hyperbranched polycarbonates**

Poly(trimethylene carbonate), (PTMC, Figure SI-1)

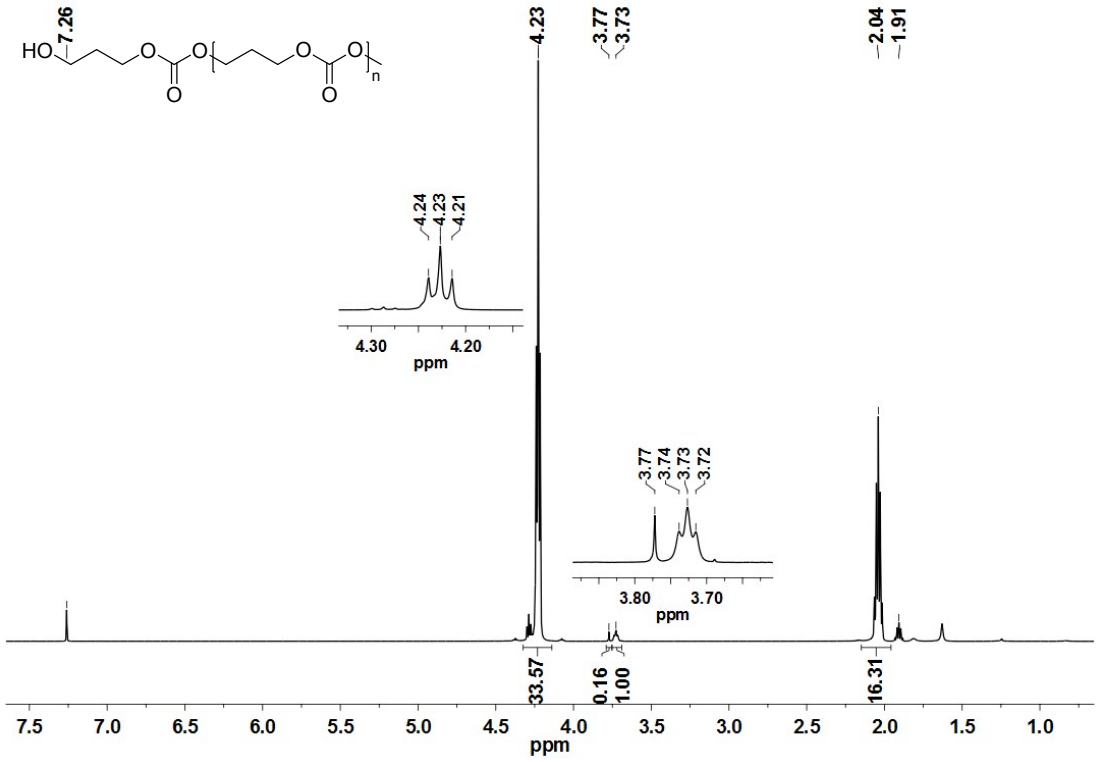


^{1}H-NMR (500 MHz, $CDCl_3$)

δ (ppm) = 2.04 (m, 2 H, $^{2}CH_2$), 3.73 (t, 2 H, $^{3}J_{HH}$ = 5.8 Hz, $^{a}CH_2$), 3.77 (s, 3 H, $O^{b}CH$), 4.23 (t, 4 H, $^{3}J_{HH}$ = 6.2 Hz, $^{1}CH_2$)

^{13}C-NMR (125 MHz, $CDCl_3$)

δ (ppm) = 28.14 (1 C, $^{2}CH_2$), 37.13 (1 C, $^{c}CH_2$), 59.01 (1 C, $^{a}CH_2$), 64.37 (2 C, $^{1}CH_2$), 65.13 (1 C, $^{d}CH_2$), 154.97 (1 C, $^{3}C_q$), 155.35 (1 C, $^{e}C_q$)



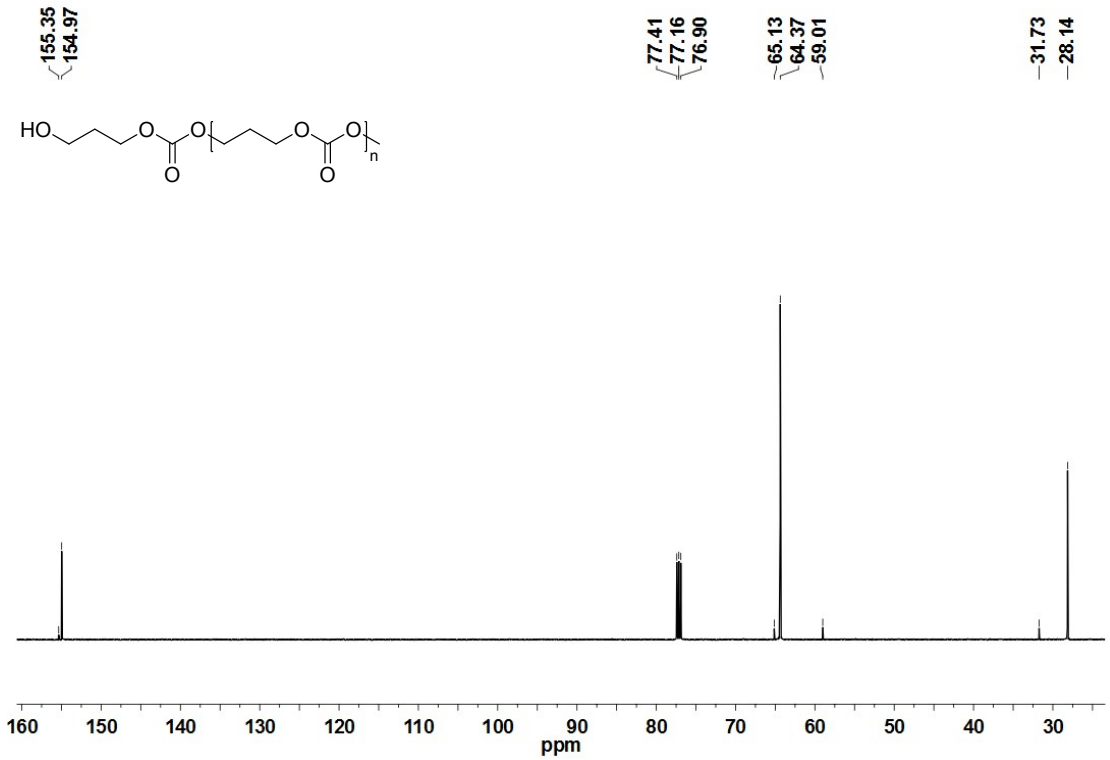
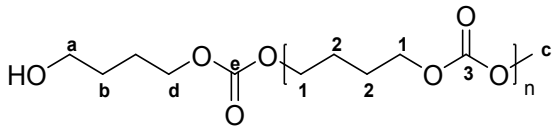


Figure SI-1. ^{1}H and ^{13}C NMR spectra of PTMC

Poly(butylene carbonate), (PBC, Figure SI-2)



^{1}H-NMR (500 MHz, $CDCl_3$)

δ (ppm) = 1.65 (m, 3 H, $^{b}CH_2$, OH), 1.76 (b, 4 H, $^{2}CH_2$), 3.67 (t, 2 H, $^{3}J_{HH}$ = 6.3 Hz, $^{a}CH_2$), 3.77 (s, 3 H, $O^{c}CH_3$), 4.15 (b, 4 H, $^{1}CH_2$)

^{13}C-NMR (125 MHz, $CDCl_3$)

δ (ppm) = 28.28 (2 C, $^{2}CH_2$), 29.04 (1 C, $^{b}CH_2$), 54.83 (1 C, $^{c}CH_3$), 62.39 (1 C, $^{a}CH_2$), 67.39 (2 C, $^{1}CH_2$), 67.89 (1 C, $^{d}CH_2$), 155.30 (1 C, $^{3}C_q$), 155.36 (1 C, $^{e}C_q$)

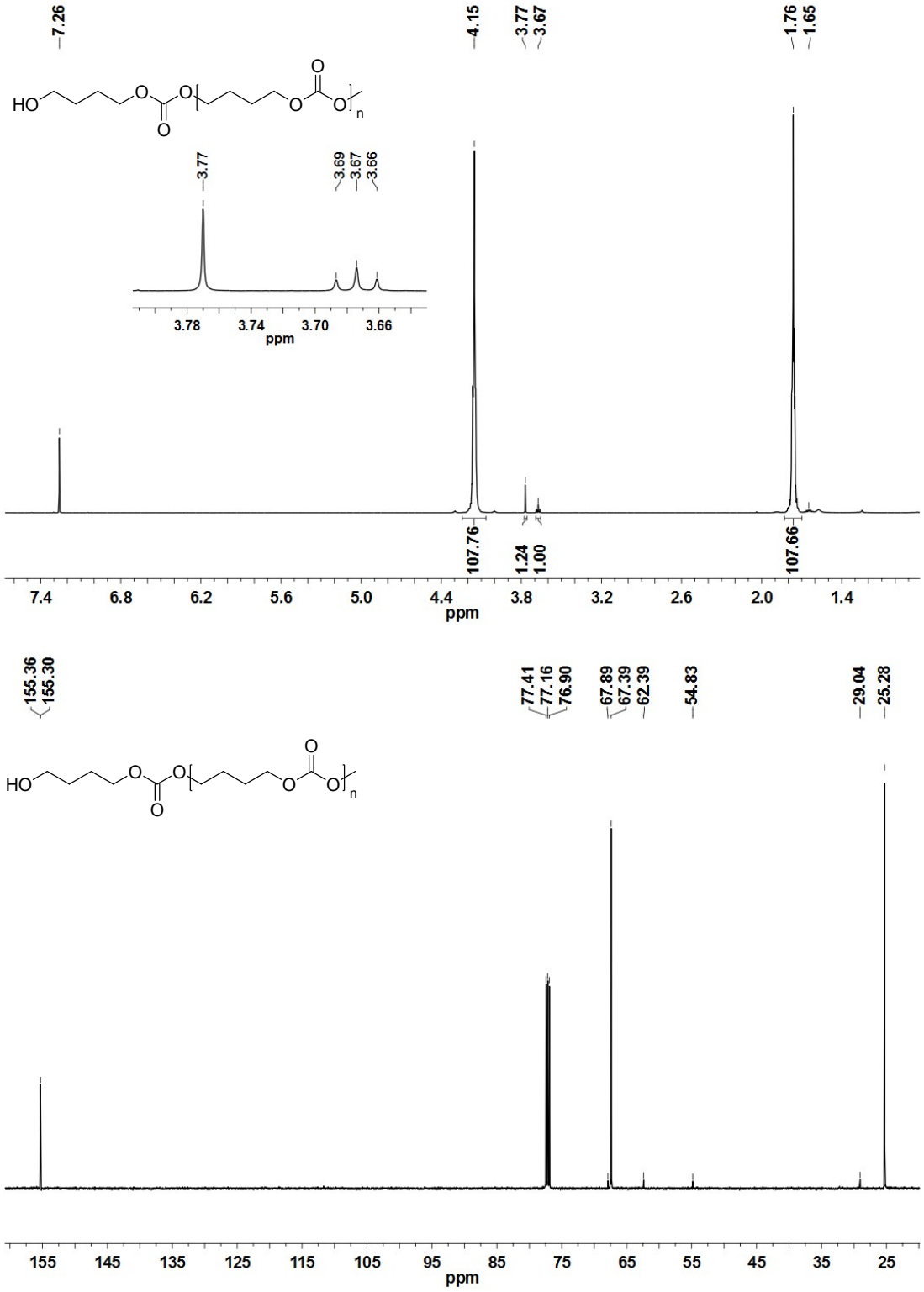
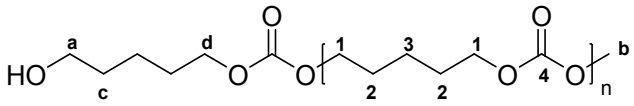


Figure SI-2. ^{1}H and ^{13}C NMR spectra of PBC

Poly(pentamethylene carbonate), (PPC, Figure SI-3)

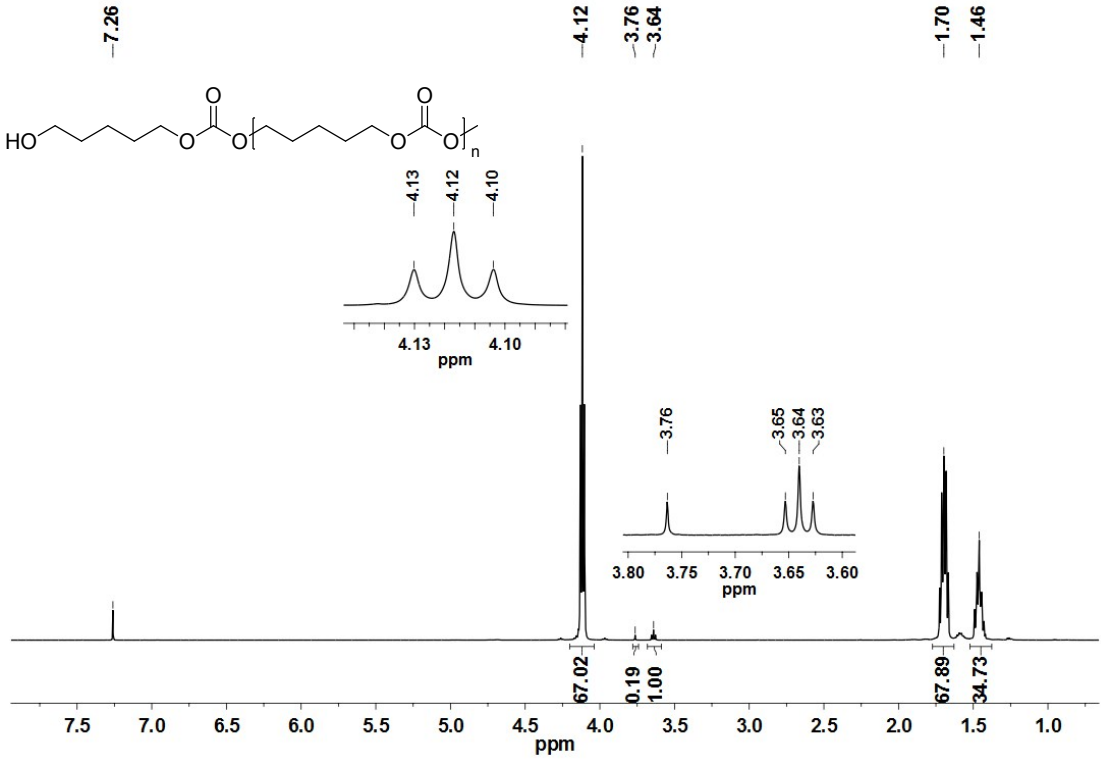


^{1}H-NMR (500 MHz, $CDCl_3$)

δ (ppm) = 1.46 (m, 2 H, $^{3}CH_2$), 1.70 (m, 4 H, $^{2}CH_2$), 3.64 (t, 2 H, $^{3}J_{HH}$ = 6.5 Hz, $^{a}CH_2$), 3.76 (s, 3 H, $O^{b}CH_3$), 4.12 (t, 4 H, $^{3}J_{HH}$ = 6.6 Hz, $^{1}CH_2$)

^{13}C-NMR (125 MHz, $CDCl_3$)

δ (ppm) = 21.97 (1 C, $^{3}CH_2$), 28.19 (2 C, $^{2}CH_2$), 32.14 (1 C, $^{c}CH_2$), 62.51 (1 C, $^{a}CH_2$), 67.50 (2 C, $^{1}CH_2$), 67.71 (1 C, $^{d}CH_2$), 155.16 (1 C, $^{4}C_q$)



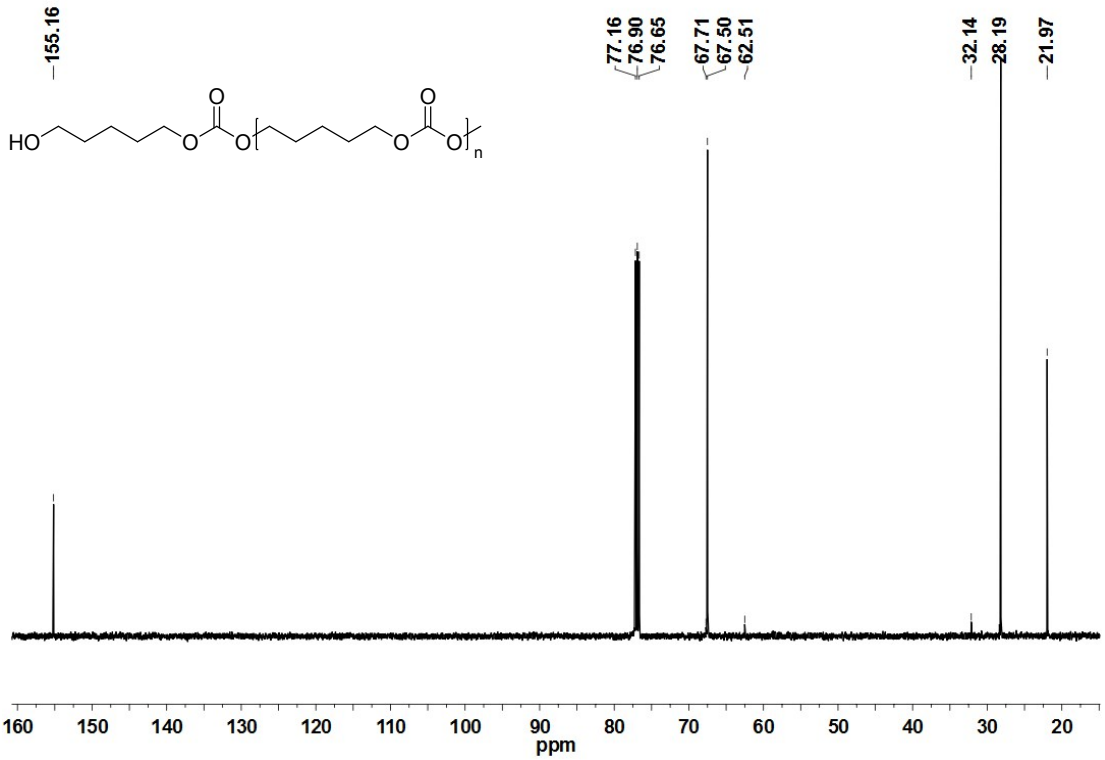
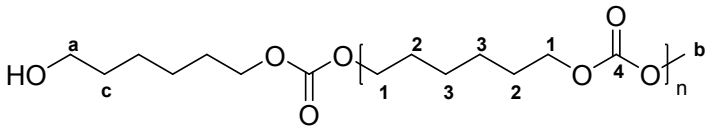


Figure SI-3. ^{1}H NMR and ^{13}C spectra of PPC

Poly(hexamethylene carbonate), (PHC, Figure SI-4)



^{1}H-NMR (500 MHz, $CDCl_3$)

δ (ppm) = 1.40 (m, 4 H, $^{3}CH_2$), 1.67 (m, 4 H, $^{2}CH_2$), 3.63 (t, 2 H, $^{3}J_{HH}$ = 6.5 Hz, $^{a}CH_2$), 3.77 (s, 3 H, $O^{b}CH_3$), 4.11 (t, 4 H, $^{3}J_{HH}$ = 6.7 Hz, $^{1}CH_2$)

^{13}C-NMR (125 MHz, $CDCl_3$)

δ (ppm) = 25.75 (2 C, $^{3}CH_2$), 28.93 (2 C, $^{2}CH_2$), 32.95 (1 C, $^{c}CH_2$), 55.00 (1 C, $^{b}CH_3$), 63.13 (1 C, $^{a}CH_2$), 68.14 (2 C, $^{1}CH_2$), 155.72 (1 C, $^{4}C_q$)

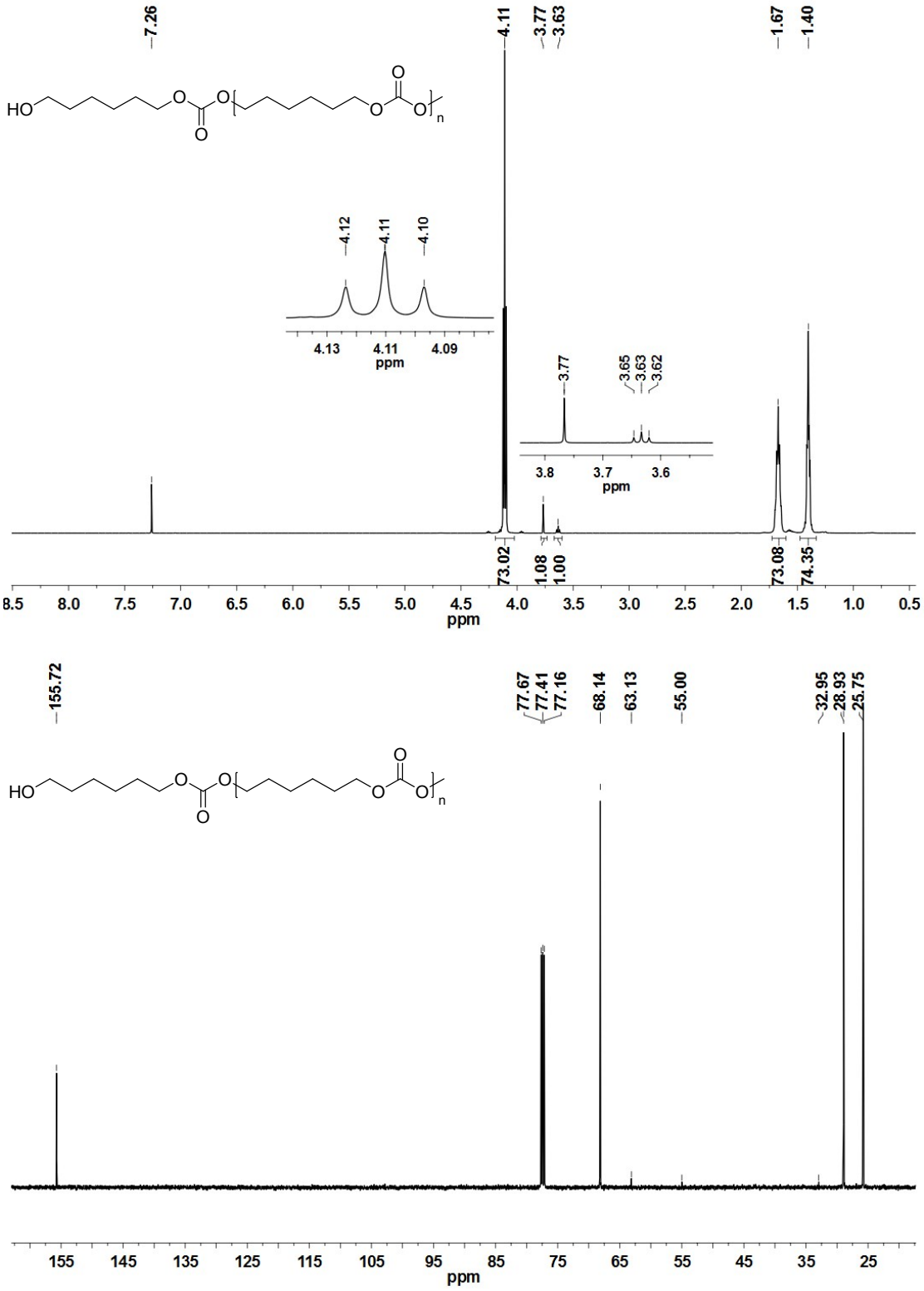
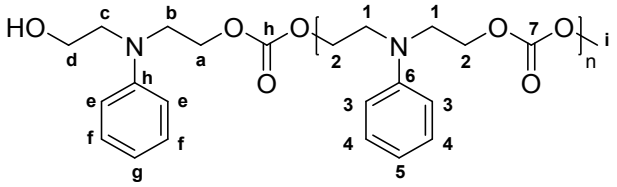


Figure SI-4. ^{1}H and ^{13}C NMR spectra of PHC

Poly(diethylphenylamine carbonate), (PDEAC, Figure SI-5)

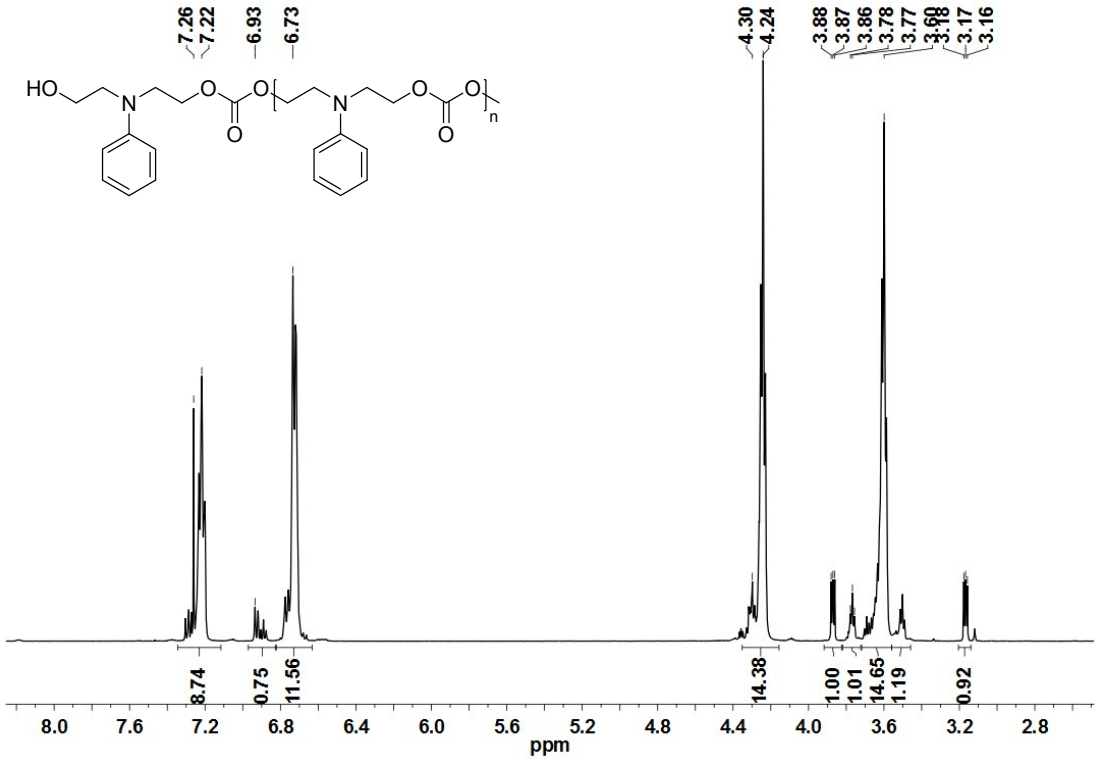


^{1}H-NMR (500 MHz, $CDCl_3$)

δ (ppm) = 3.17 (t, 2 H, $^{3}J_{HH}$ = 4.8 Hz, $^{b}CH_2$), 3.54-3.70 (m, 4 H, $^{1}CH_2$), 3.50 (t, 2 H, $^{3}J_{HH}$ = 5.6 Hz, $^{c}CH_2$), 3.77 (t, 2 H, $^{3}J_{HH}$ = 5.6 Hz, $^{d}CH_2$), 3.87 (t, 2 H, $^{3}J_{HH}$ = 4.8 Hz, $^{a}CH_2$), 4.17-4.40 (m, 4 H, $^{2}CH_2$), 6.66-6.80 (m, 3 H, $^{3,5}CH$), 6.86-6.94 (m, 3 H, $^{e,g}CH$), 7.16-7.26 (m, 2 H, ^{4}CH), 7.26-7.31 (m, 2 H, ^{f}CH)

^{13}C-NMR (125 MHz, $CDCl_3$)

δ (ppm) = 49.52 (1 C, $^{b}CH_2$), 49.79 (2 C, $^{1}CH_2$), 50.64 (1 C, $^{c}CH_2$), 54.50 (1 C, $^{i}CH_3$), 60.30 (1 C, $^{d}CH_2$), 64.91 (2 C, $^{2}CH_2$), 67.07 (1 C, $^{a}CH_2$), 112.29, 117.44, 129.65, 147.06 (6 C, $^{3\text{-}6}C_{Ar}$), 113.08, 115.85, 120.17, 129.31, 129.53, 147.92 (6 C, $^{e,f,g,h}C_{Ar}$), 155.15 (1 C, $^{7}C_q$), 155.21 (1 C, $^{h}C_q$)



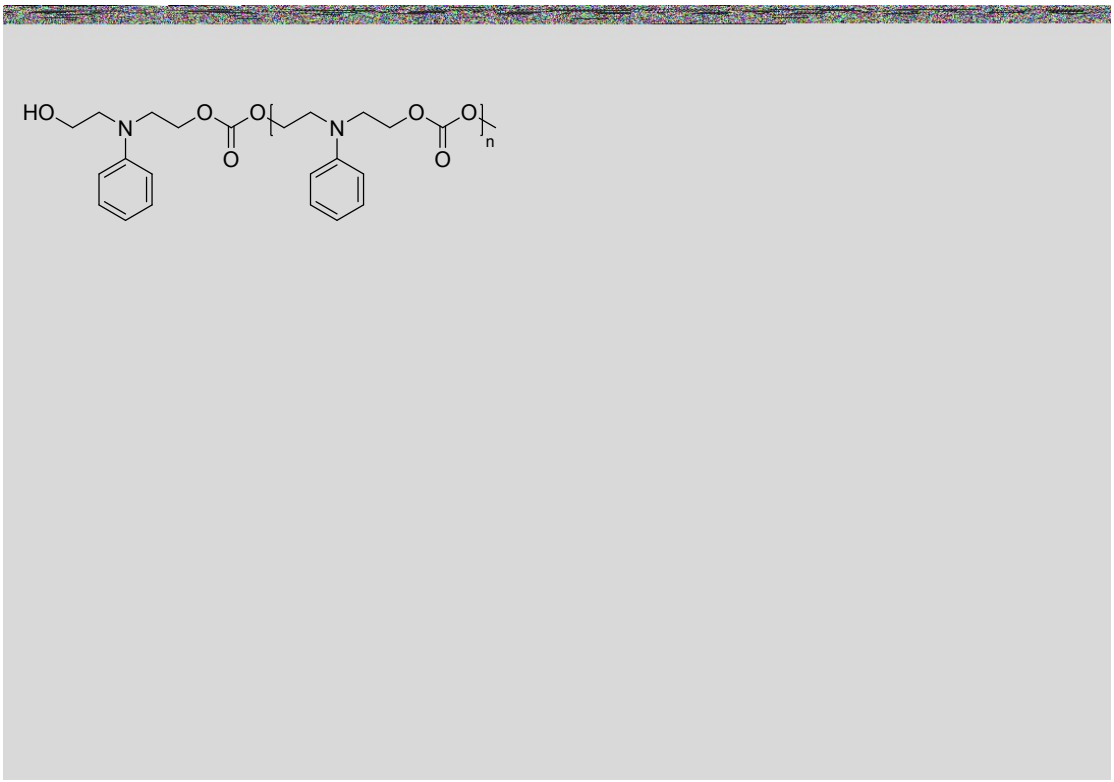
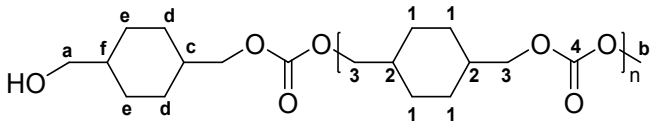


Figure SI-5. ^{1}H and ^{13}C NMR spectra of PDEAC

Poly(cyclohexan-1,4-dimethylene carbonate), (PCDMC, Figure SI-6)



^{1}H-NMR (500 MHz, $CDCl_3$)

δ (ppm) = 0.97-1.90 (m, 10 H, $^{1}CH_2$, ^{2}CH), 3.44-3.54 (m, 2 H, $^{a}CH_2$), 3.77 (s, 3 H, $O^{b}CH_3$), 3.93-4.04 (m, 4 H, $^{3}CH_2$)

^{13}C-NMR (125 MHz, $CDCl_3$)

δ (ppm) = 25.18, 28.64 (4 C, $^{1}CH_2$), 25.41 (2 C, $^{d}CH_2$), 28.90 (2 C, $^{e}CH_2$), 34.56, 37.12 (2 C, ^{2}CH), 37.39 (1 C, ^{c}CH), 40.42 (1 C, ^{f}CH), 54.72 (1 C, $^{b}CH_3$), 68.74, (1 C, $^{a}CH_2$), 70.66, 72.80 (2 C, $^{3}CH_2$), 155.55 (1 C, $^{4}C_q$)

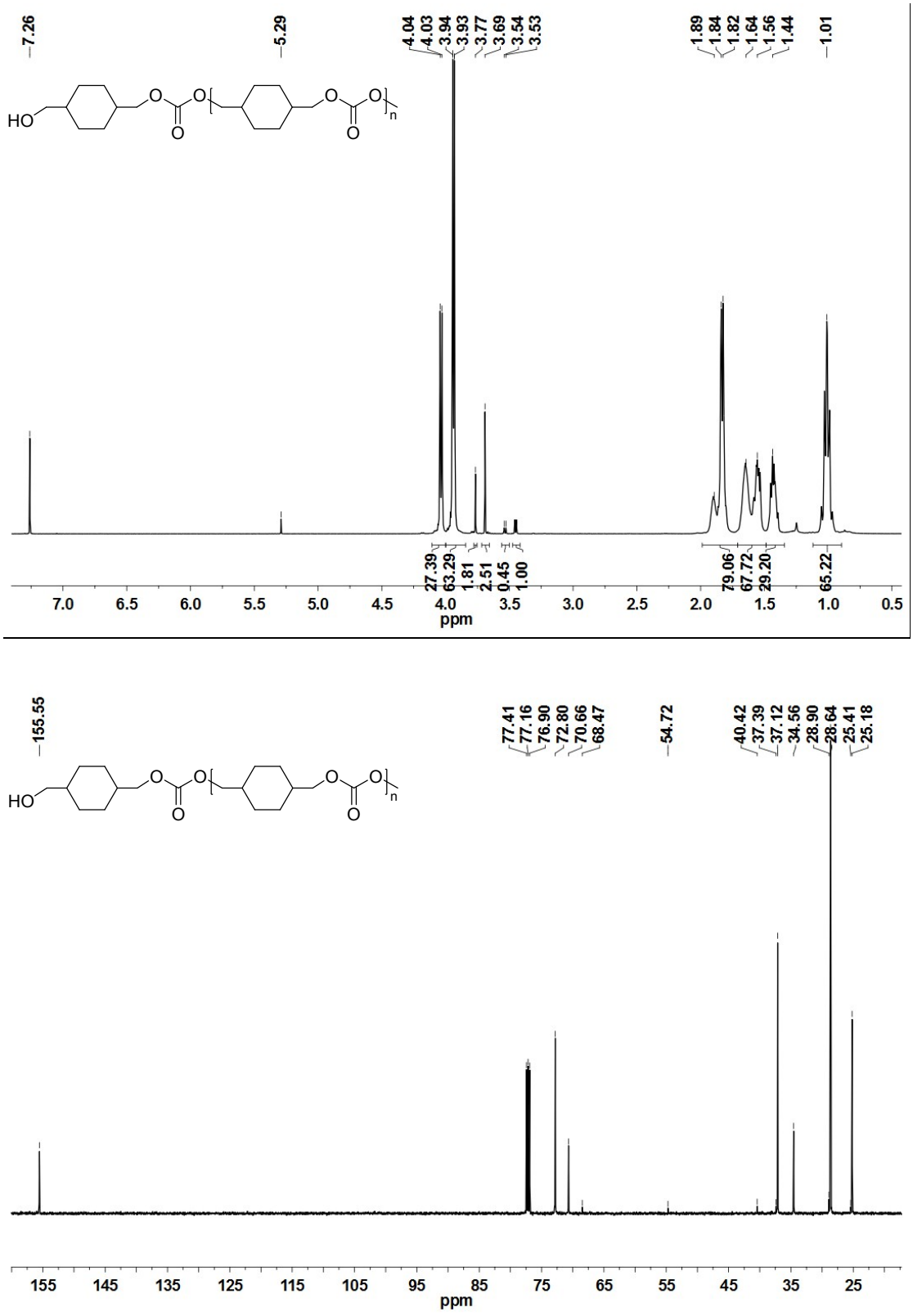
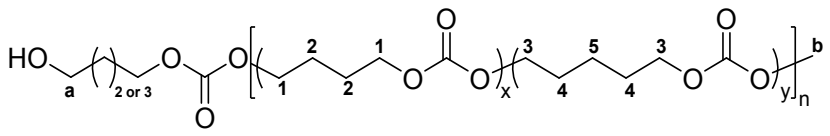


Figure SI-6. ^{1}H and ^{13}C NMR spectra of PCDMC

Poly(butylene carbonate)-*co*-poly(pentamethylene carbonate), (PBC-*co*-PPC, Figure SI-7)



^{1}H-NMR (500 MHz, $CDCl_3$)

δ (ppm) = 1.46 (m, 2 H, $^{5}CH_2$), 1.63-1.73 (m, 4 H, $^{4}CH_2$), 1.76 (m, 4 H, $^{2}CH_2$), 3.67 (m, 2 H, $^{a}CH_2$), 3.77 (s, 3 H, $O^{b}CH_3$), 4.10-4.20 (m, 4 H, $^{1}CH_2$; 4 H, $^{3}CH_2$)

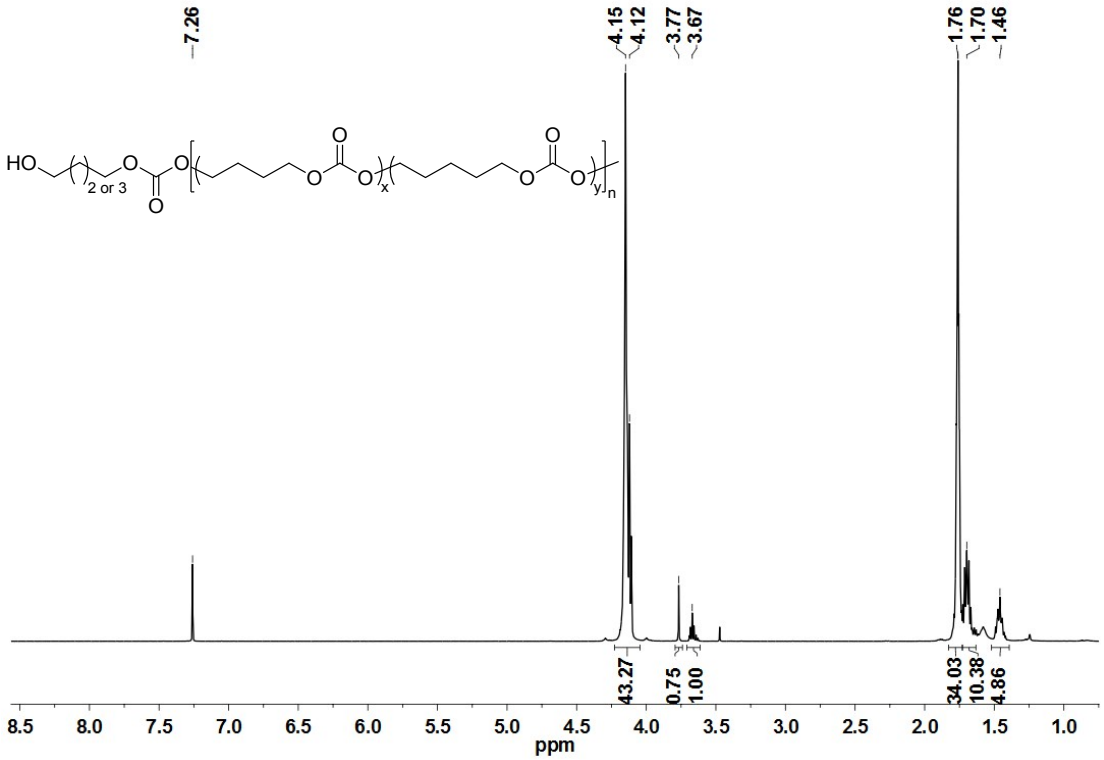
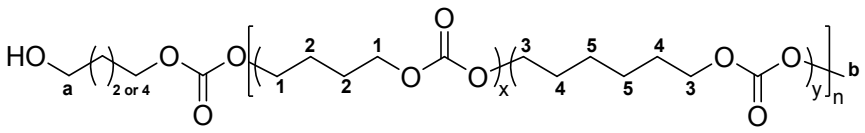


Figure SI-7. ^{1}H NMR spectrum of PBC-*co*-PPC

Poly(butylene carbonate)-*co*-poly(hexamethylene carbonate), (PBC-*co*-PHC, Figure SI-8)



^{1}H-NMR (500 MHz, $CDCl_3$)

δ (ppm) = 1.40 (m, 4 H, $^{5}CH_2$), 1.67 (m, 4 H, $^{4}CH_2$), 1.77 (m, 4 H, $^{2}CH_2$), 3.62-3.69 (m, 2 H, $^{a}CH_2$), 3.77-3.78 (m, 3 H, O$^{b}CH_3$), 4.00-4.27 (m, 4 H, $^{1}CH_2$; 4 H, $^{3}CH_2$)

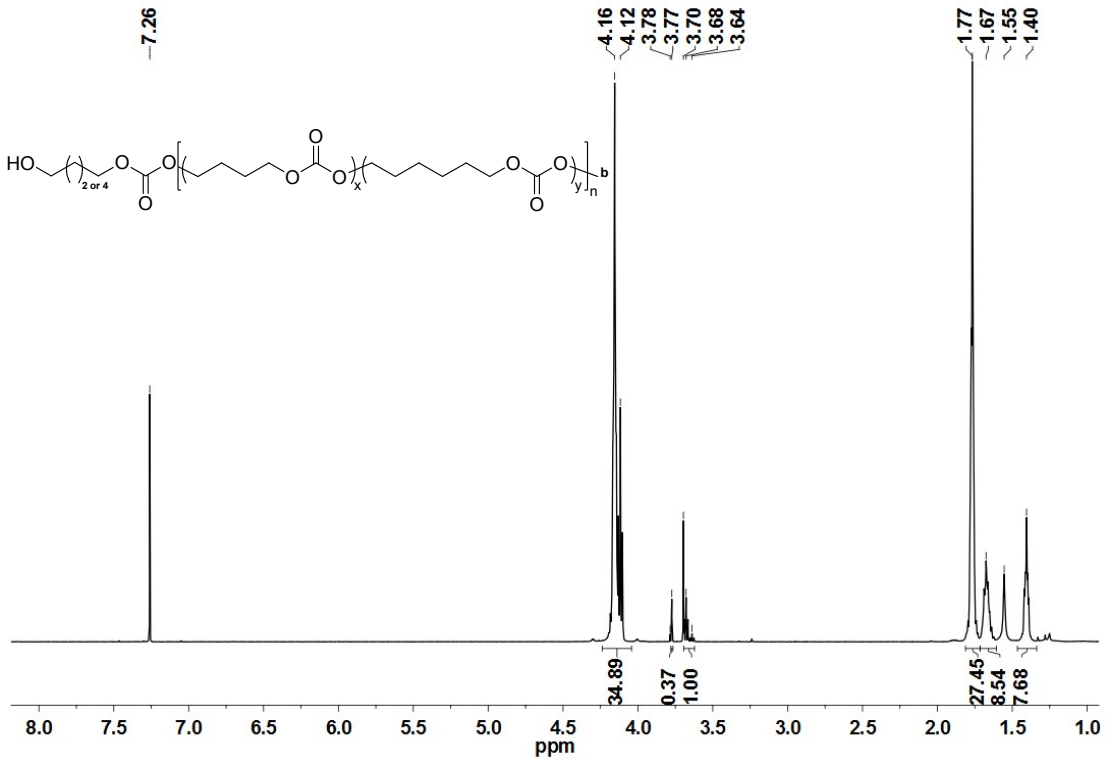
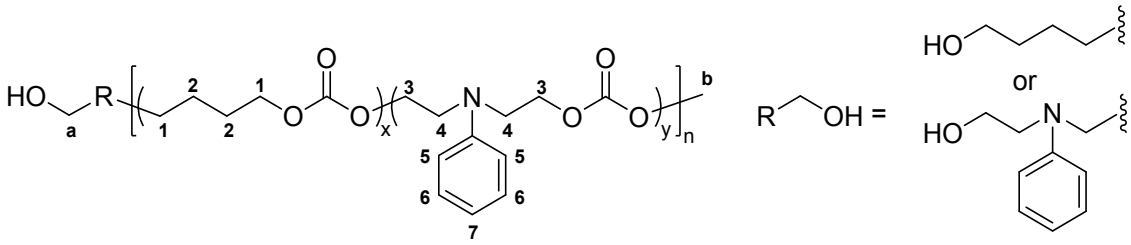


Figure SI-8. ^{1}H NMR spectrum of PBC-*co*-PHC

Poly(butylene carbonate)-*co*-poly(diethylphenylamine carbonate), (PBC-*co*-PDEAC, Figure SI-9)



^{1}H-NMR (500 MHz, $CDCl_3$)

δ (ppm) = 1.75 (m, 4 H, $^{2}CH_2$), 3.65 (m, 2 H, $^{a}CH_2$), 3.76 (b, 3 H, $O^{b}CH_3$), 4.14 (m, 4 H, $^{1}CH_2$), 4.26 (m, 4 H, $^{3}CH_2$), 6.73 (m, 3 H, $^{5,7}CH$), 7.21(m, 2 H, ^{6}CH)

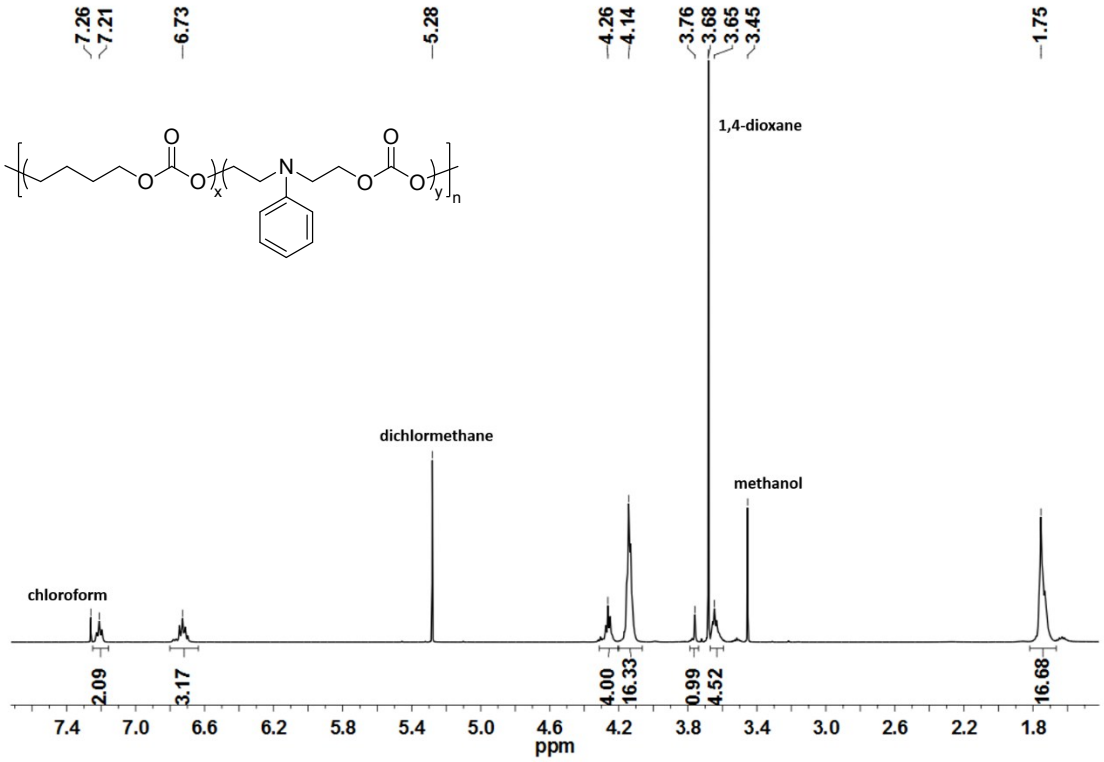
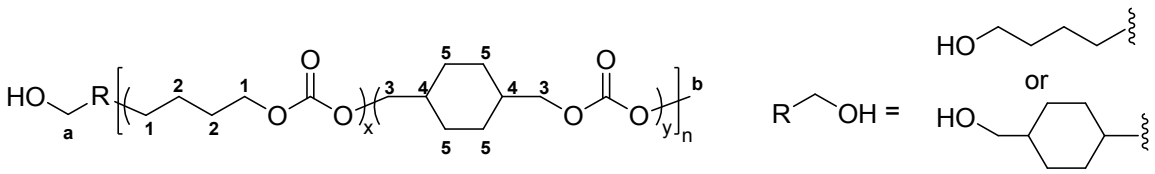


Figure SI-9. ^{1}H NMR spectrum of PBC-*co*-PDEAC

Poly(butylene carbonate)-*co*-poly(cyclohexan-1,4-dimethylene carbonate), (PBC-*co*-PCDMC, Figure SI-10)



^{1}H-NMR (500 MHz, $CDCl_3$)

δ (ppm) = 0.90-1.90 (m, 4 H, $^{2}CH_2$; 10 H, ^{4}CH, $^{5}CH_2$), 3.66 (t, $^{3}J_{HH}$ = 7.3 Hz, 2 H, $^{a}CH_2$), 3.75 (b, 3 H, $O^{b}CH_3$), 3.90-4.05 (m, 4 H, $^{3}CH_2$), 4.14 (m, 4 H, $^{1}CH_2$)

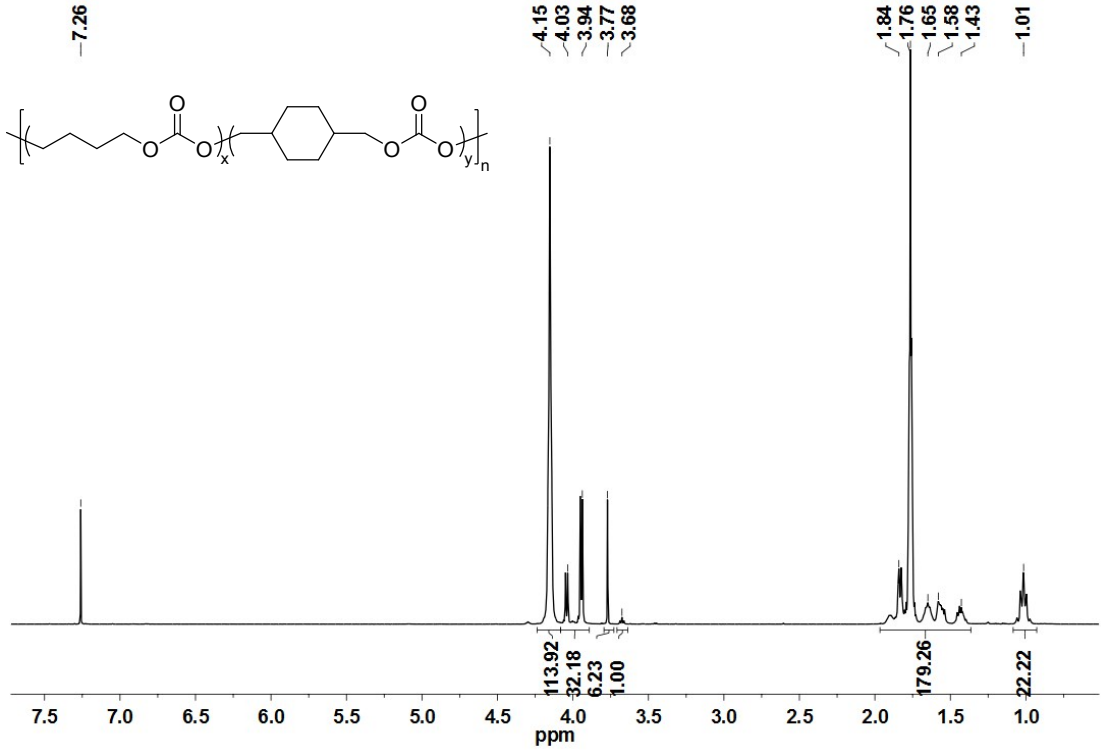


Figure SI-10. ^{1}H NMR spectrum of PBC-*co*-PCDMC

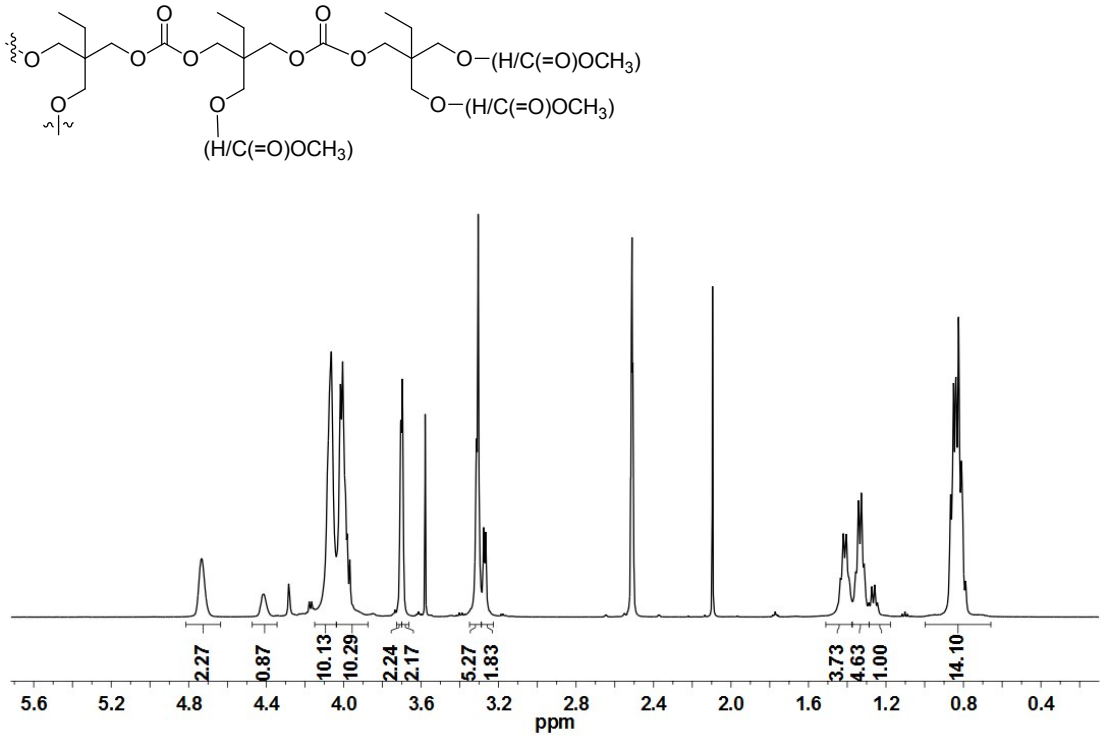


Figure SI-11. ^{1}H NMR spectrum of PTHPC

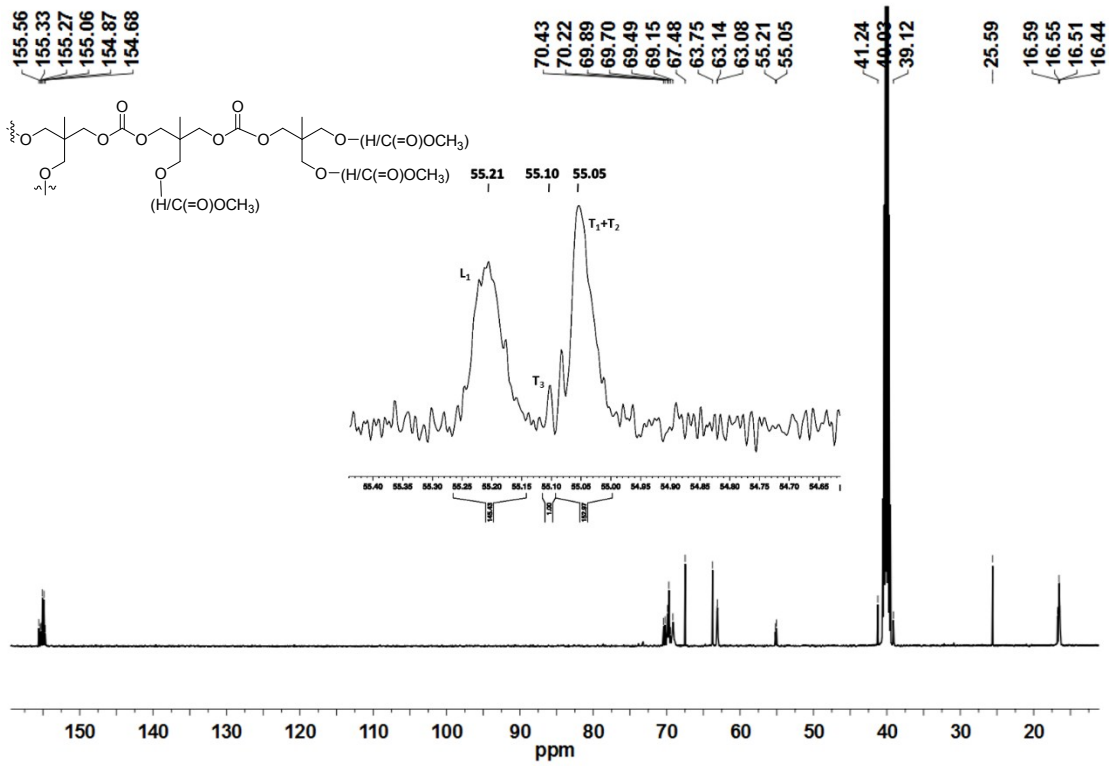


Figure SI-12. ^{13}C NMR spectrum of PTHEC 1

- **Detailed ESI-MS spectrum and analysis of PBC 9**

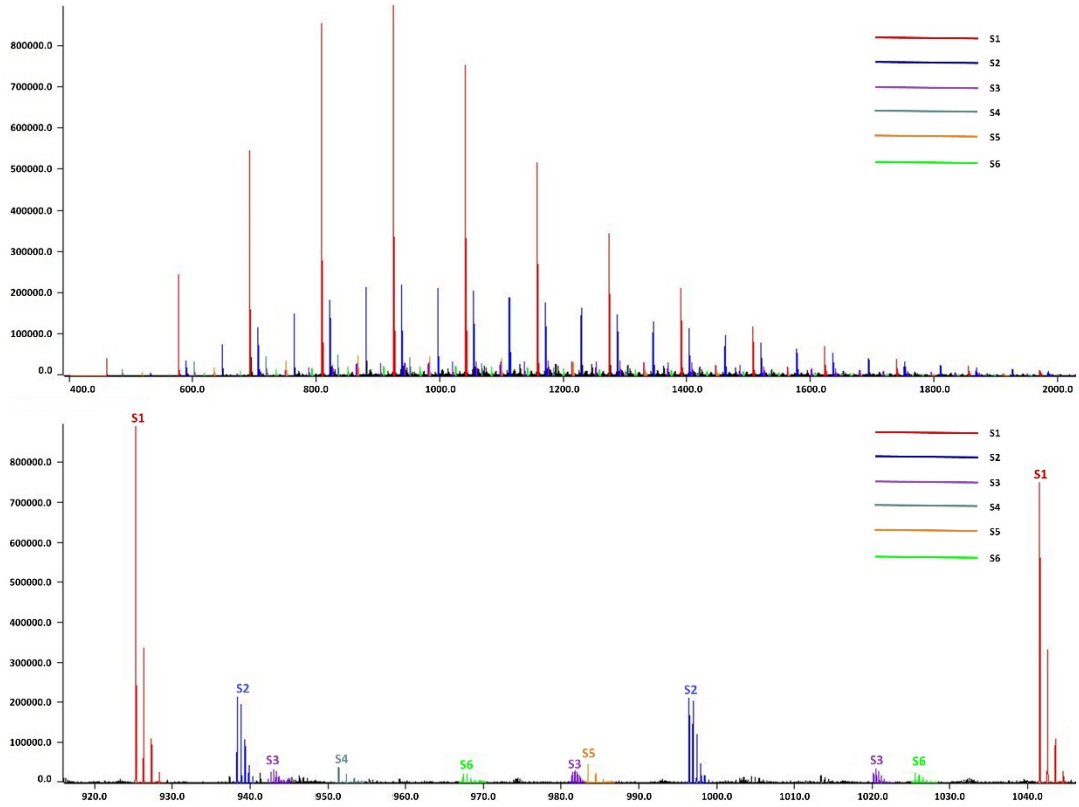
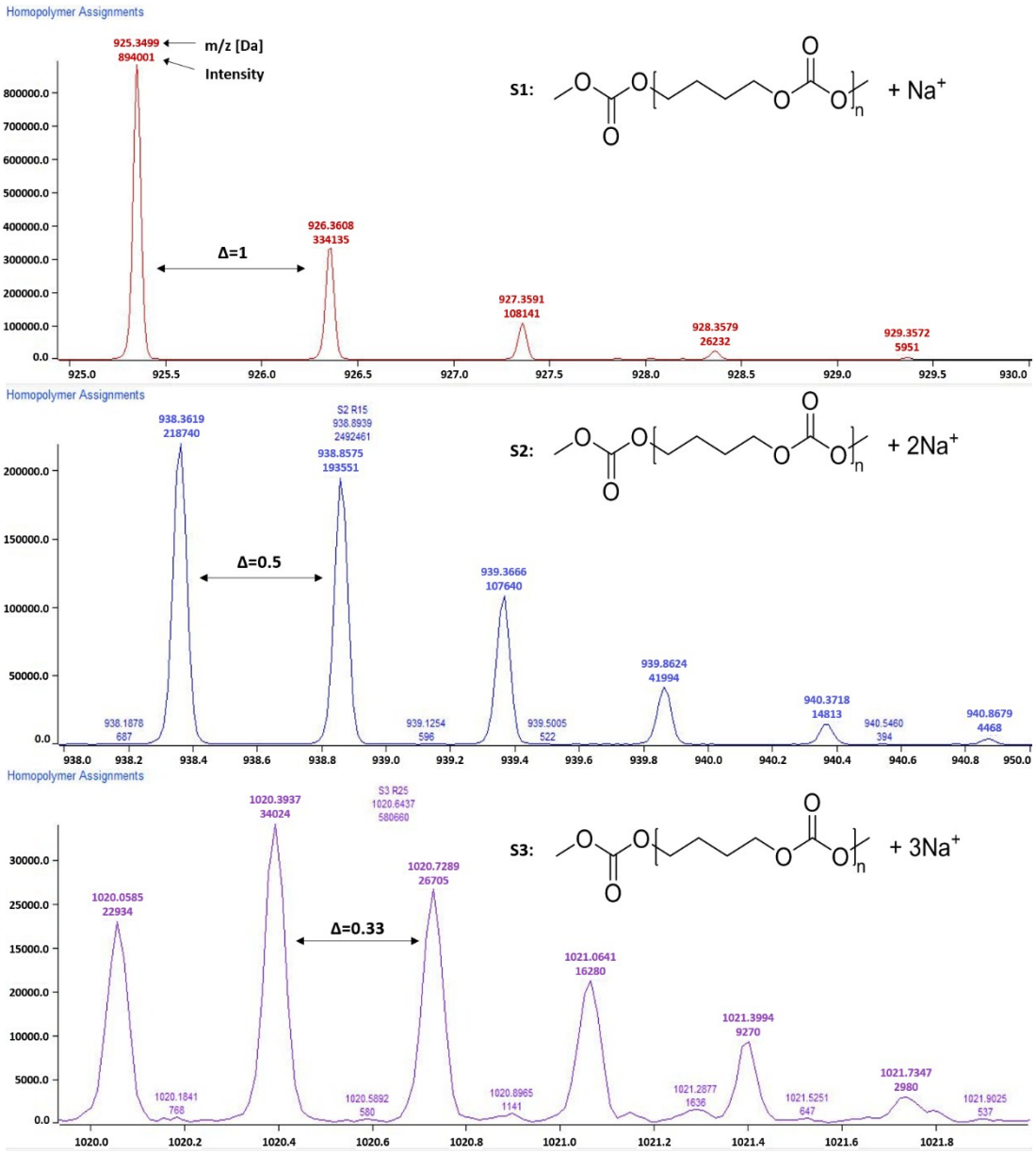


Figure SI-13. Whole spectrum of PBC 9 in the m/z region of 400 to 2000.


Homopolymer Assignments
925.3499
894001
m/z [Da]
Intensity
926.3608
334135
Δ=1
927.3591
108141
928.3579
26232
929.3572
5951
S1:
+ Na+
Homopolymer Assignments
938.3619
218740
S2 R15
938.8939
2492461
938.8575
193551
Δ=0.5
939.3666
107640
939.8624
41994
940.3718
14813
940.8679
4468
938.1878
687
939.1254
596
939.5005
522
940.5460
394
S2:
+ 2Na+
Homopolymer Assignments
1020.3937
34024
S3 R25
1020.6437
580660
1020.7289
26705
1020.0585
22934
Δ=0.33
1021.0641
16280
1021.3994
9270
1021.7347
2980
1020.1841
768
1020.5892
580
1020.8965
1141
1021.2877
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1021.5251
647
1021.9025
537
S3:
+ 3Na+

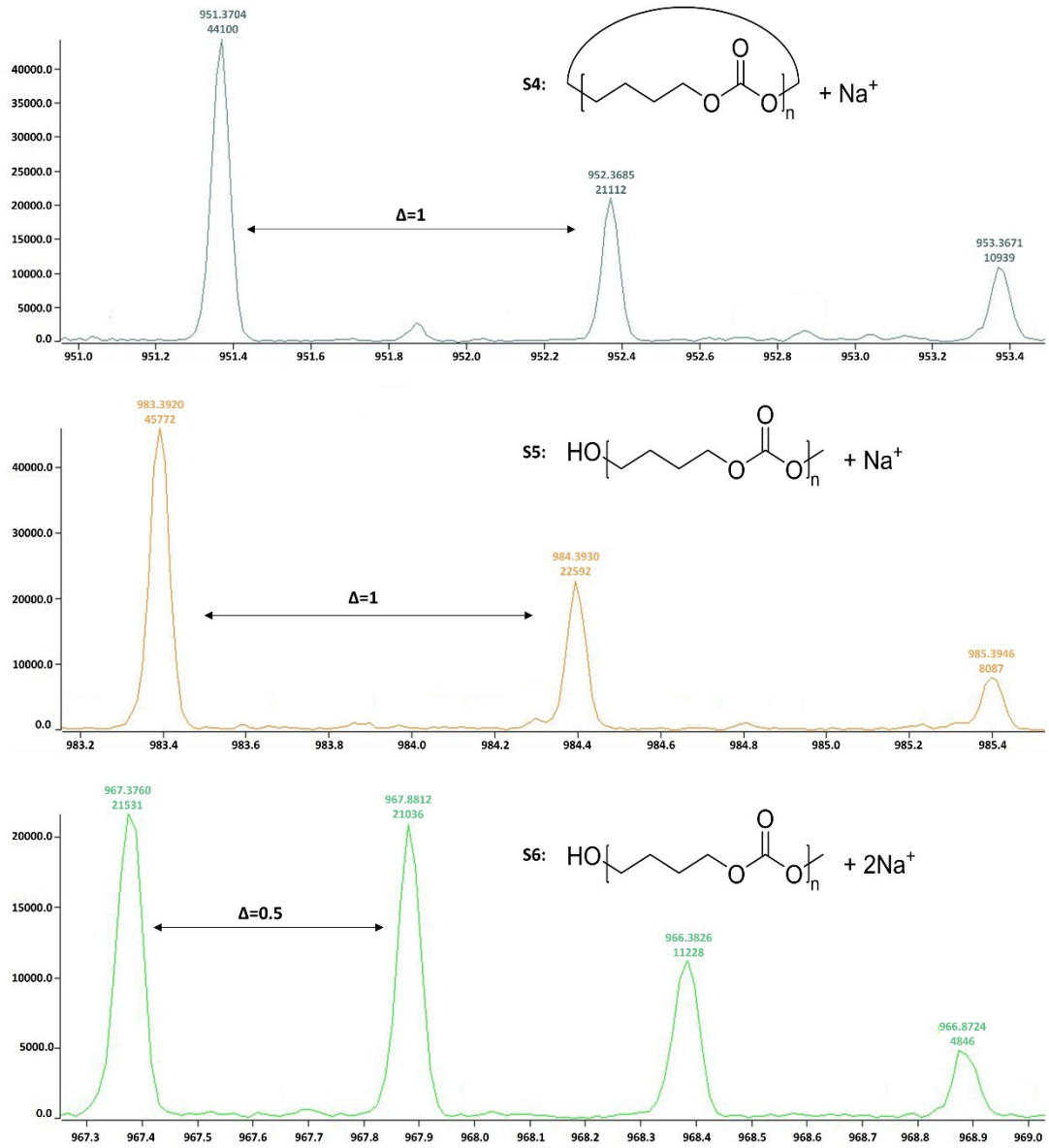

Figure SI-14. Detailed analysis of ESI-MS spectrum of PBC 9 (S1-S6)

- **Hydrolytic degradation investigation of PBC specimen at 37 °C pH = 7.4 and 55 °C pH = 13.0**

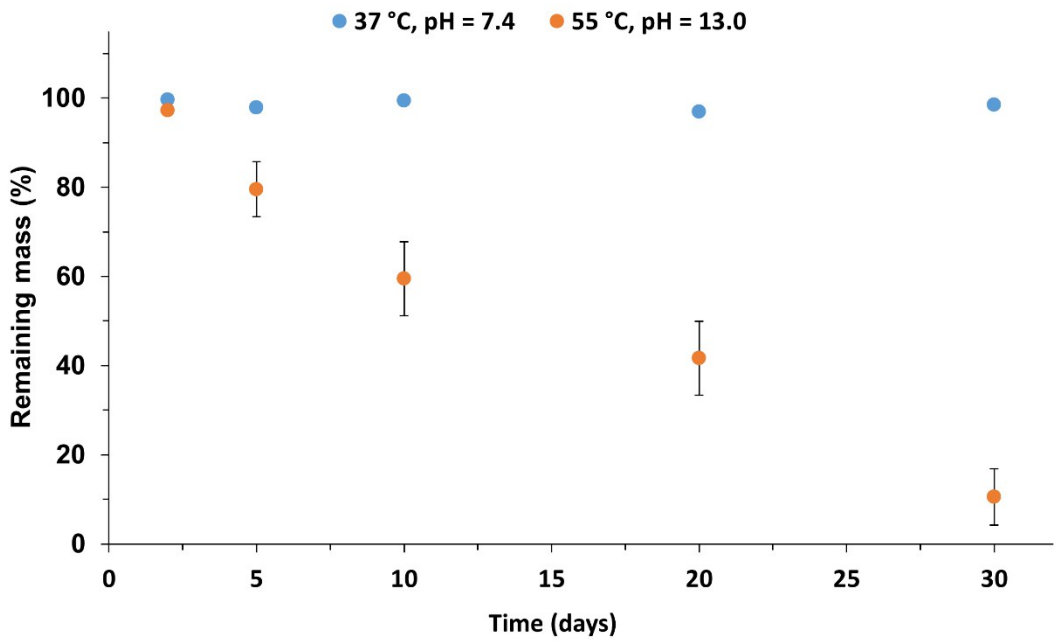

Figure SI-15. Mass loss of PBC specimen during 30 days under biological and accelerated conditions, i.e., 37 °C pH = 7.4 and 55 °C pH = 13.0.