SUPPORTING INFORMATION

MALDI-TOF/TOF CID Study of Poly(Butylene Adipate) Fragmentation Reactions

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FIGURE CAPTIONS:

Figure S1. Medium effective kinetic energy (collision gas pressure: 1.5 × 10^{-6} Torr) MALDI-TOF/TOF mass spectrum of dibutanol terminated poly(butylene adipate) (Str. 1-E1 Li+, 1497.8 Da); covering the monomeric (A: 70–390 Da), dimeric through trimeric (B: 390–790 Da), and tetrameric through pentameric (C: 790–1190 Da) mass regions.

Figure S2. MALDI-TOF/TOF mass spectrum for cyclic PBA structure 1-CyE at a *low* collision gas pressure of 1.5 × 10^{-6} Torr. Precursor ion (1023.5 Da) is through Na+ cationization.

Figure S3. MALDI-TOF/TOF mass spectrum for linear butanol-carboxyl terminated PBA structure 1-E2 at a *low* collision gas pressure of 1.5 × 10^{-6} Torr. Precursor ion (1041.5 Da) is through Na+ cationization.

Figure S4. MALDI-TOF/TOF mass spectrum for linear butanol-carboxyl terminated PBA structure, with an extra sodium atom (Str. 1-E2Na), at a *low* collision gas pressure of 1.5 × 10^{-6} Torr. Precursor ion (1063.5 Da) is through Na+ cationization.

Figure S5. MALDI-TOF/TOF mass spectrum for linear butanol-carboxyl terminated PBA structure, with and extra lithium atom (Str. 1-E2Li), at a *low* collision gas pressure of 1.5 × 10^{-6} Torr. Precursor ion (1031.5 Da) is through Li+ cationization.

Figure S6. MALDI-TOF/TOF mass spectrum for linear carboxyl-carboxyl terminated PBA structure 1-E3 at a *low* collision gas pressure of 1.5 × 10^{-6} Torr. Precursor ion (753.4 Da) is through Li+ cationization.

Figure S7. MALDI-TOF/TOF mass spectrum for linear butanol-ethanol terminated PBA structure 1-E4 at a *low* collision gas pressure of 1.5×10^{-6} Torr. Precursor ion (1085.6 Da) is through Na+ cationization.

Figure S1.

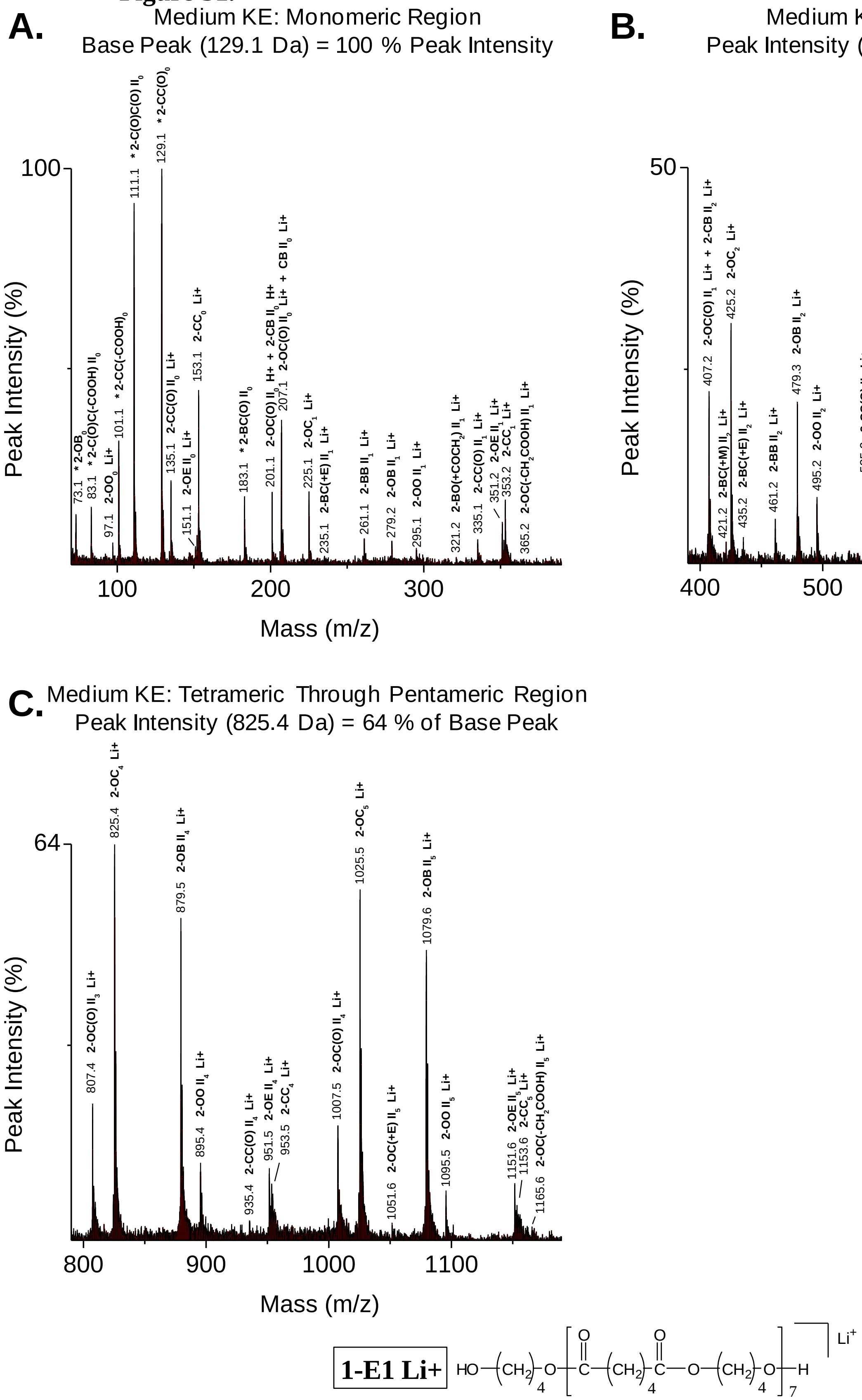
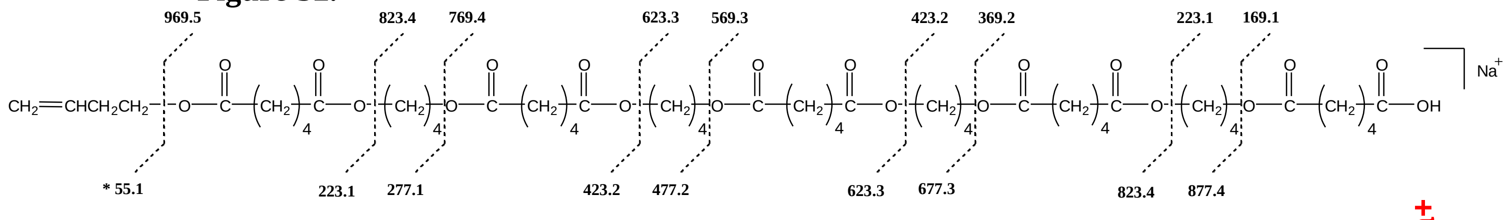

A.
Medium KE: Monomeric Region
Base Peak (129.1 Da) = 100 % Peak Intensity
B.
Medium KE: Dimeric/Trimer Region
Peak Intensity (625.3 Da) = 50 % of Base Peak
C.
Medium KE: Tetrameric Through Pentameric Region
Peak Intensity (825.4 Da) = 64 % of Base Peak
Peak Intensity (%)
Mass (m/z)
1-E1 Li+

Figure S2.



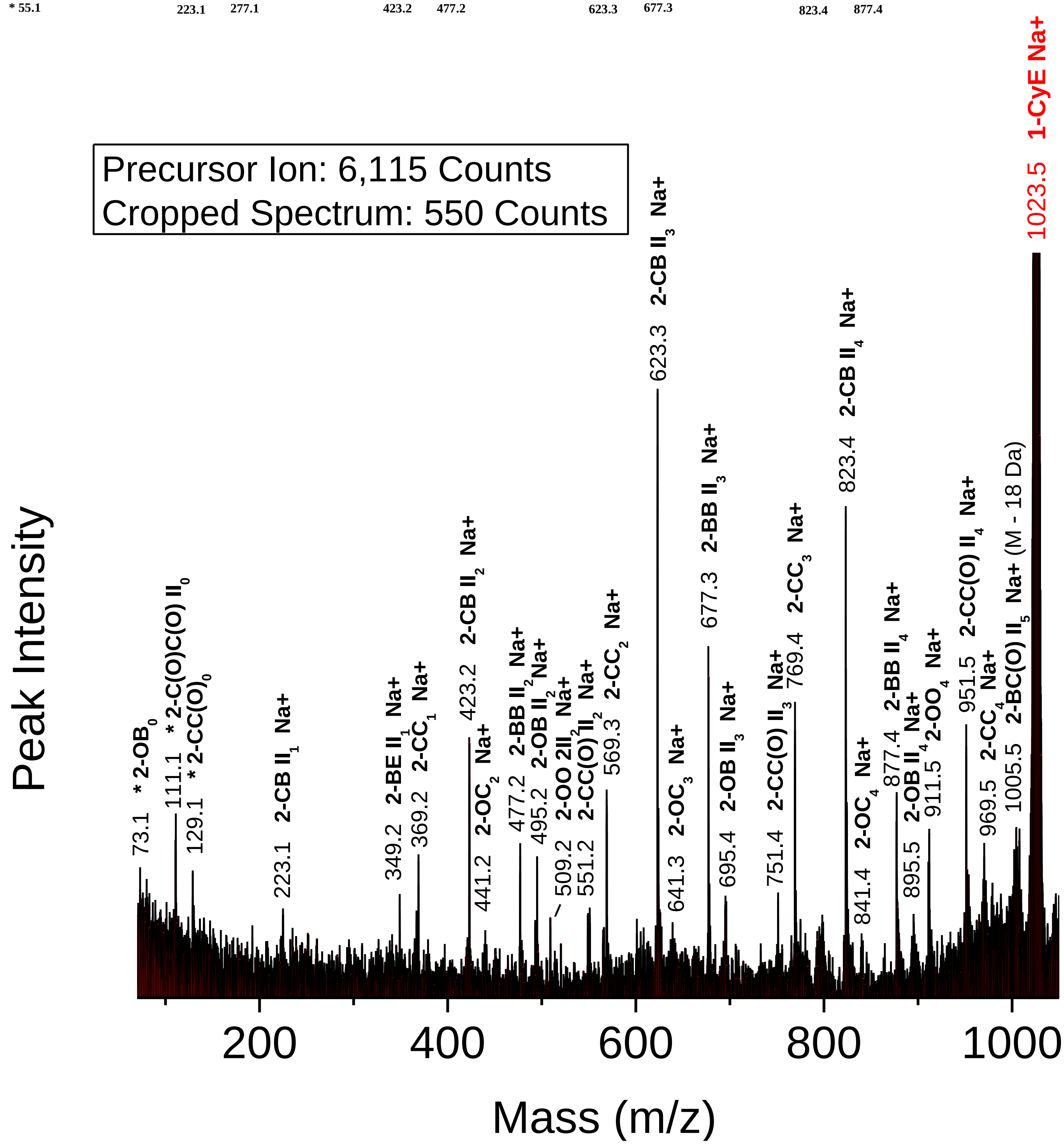
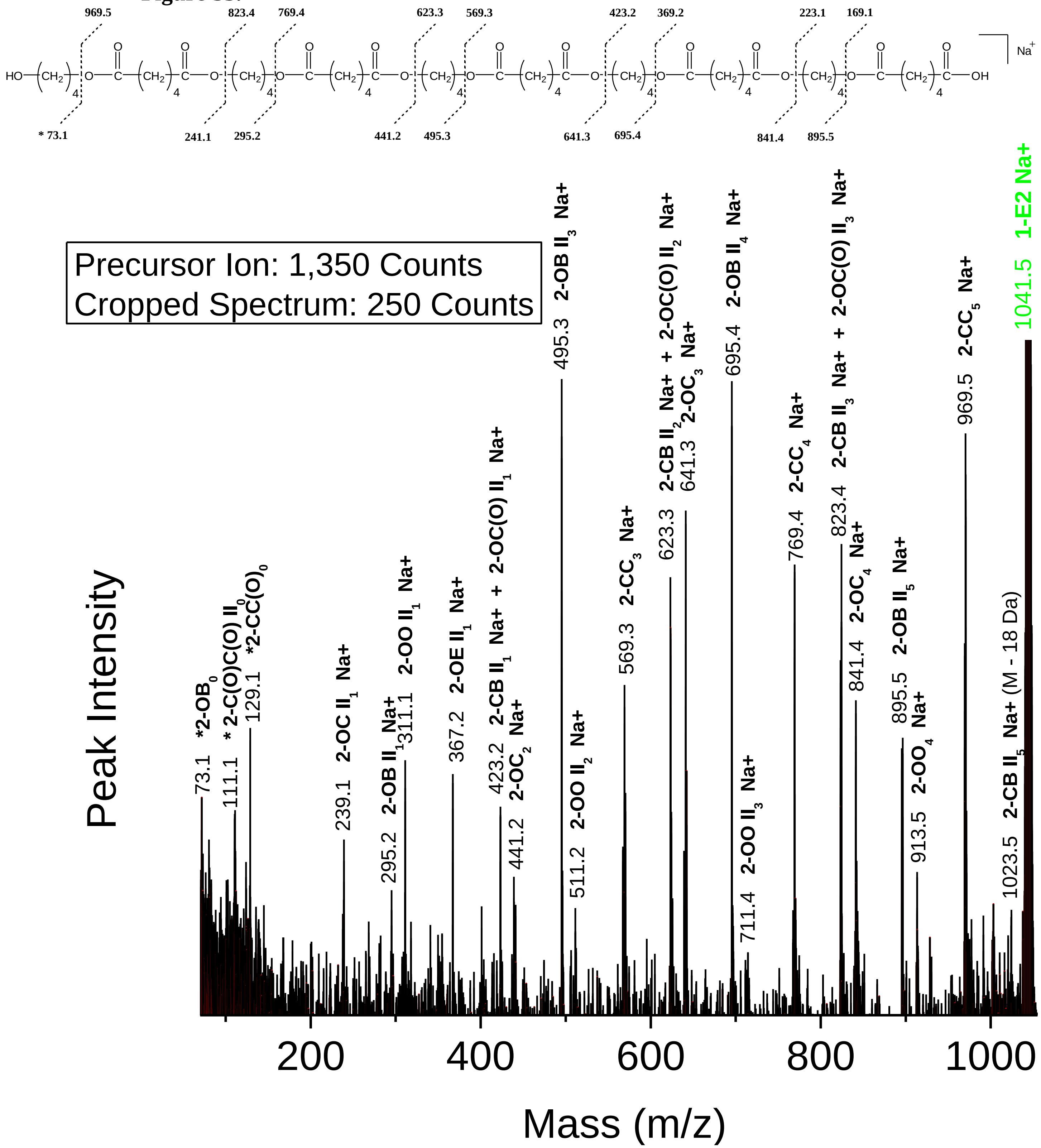
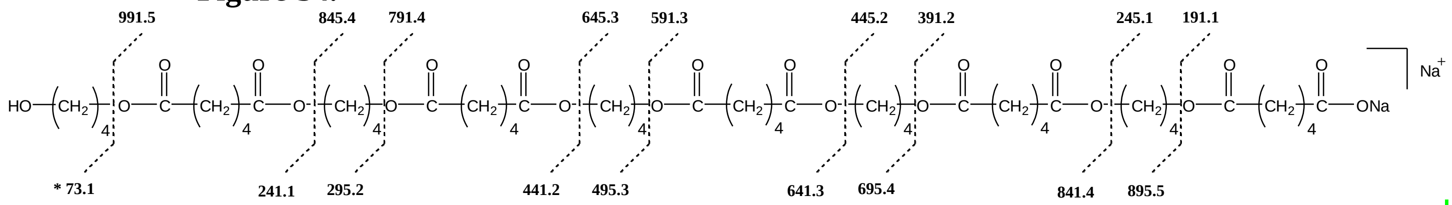

Precursor Ion: 6,115 Counts
Cropped Spectrum: 550 Counts
Peak Intensity
Mass (m/z)
1023.5 1-CyE Na+
623.3 2-CB II3 Na+
823.4 2-CB II4 Na+
677.3 2-BB II3 Na+
423.2 2-CB II2 Na+
769.4 2-CC3 Na+
951.5 2-CC(O) II4 Na+
1005.5 2-BC(O) II5 Na+ (M - 18 Da)

Figure S3.


Precursor Ion: 1,350 Counts
Cropped Spectrum: 250 Counts
Peak Intensity
Mass (m/z)
1041.5 1-E2 Na+
969.5 2-CC5 Na+
1023.5 2-CB II5 Na+ (M - 18 Da)
913.5 2-OO4 Na+
895.5 2-OB II5 Na+
841.4 2-OC4 Na+
823.4 2-CB II3 Na+ + 2-OC(O) II3 Na+
769.4 2-CC4 Na+
711.4 2-OO II3 Na+
695.4 2-OB II4 Na+
641.3 2-OC3 Na+
623.3 2-CB II2 Na+ + 2-OC(O) II2 Na+
569.3 2-CC3 Na+
511.2 2-OO II2 Na+
495.3 2-OB II3 Na+
441.2 2-OC2 Na+
423.2 2-CB II1 Na+ + 2-OC(O) II1 Na+
367.2 2-OE II1 Na+
311.1 2-OO II1 Na+
295.2 2-OB II1 Na+
239.1 2-OC II1 Na+
129.1 *2-CC(O)0
111.1 * 2-C(O)C(O) II0
73.1 *2-OB0
200
400
600
800
1000

Electronic Supplementary Material (ESI) for RSC Advances

Figure S4.



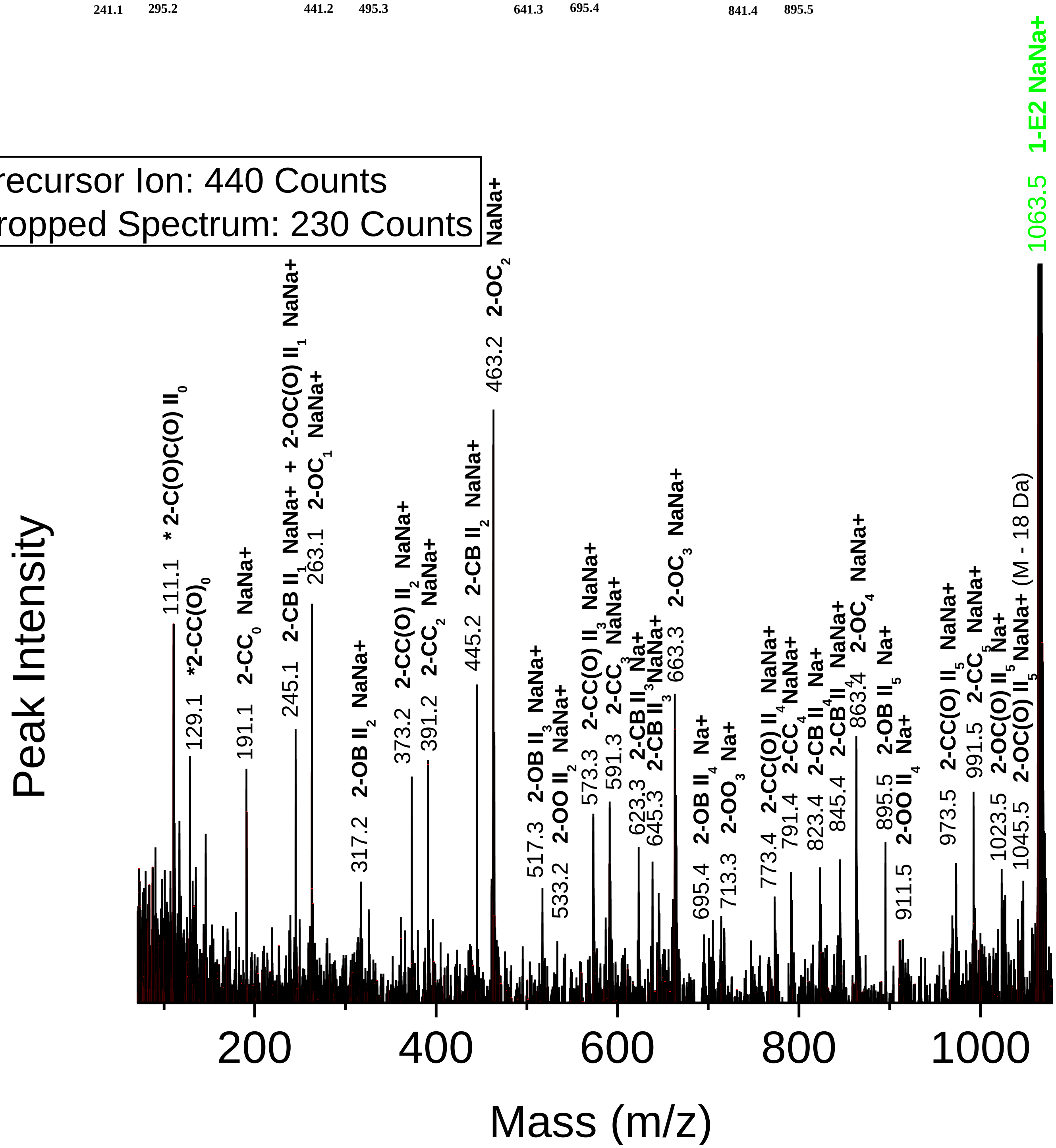


Figure S5.

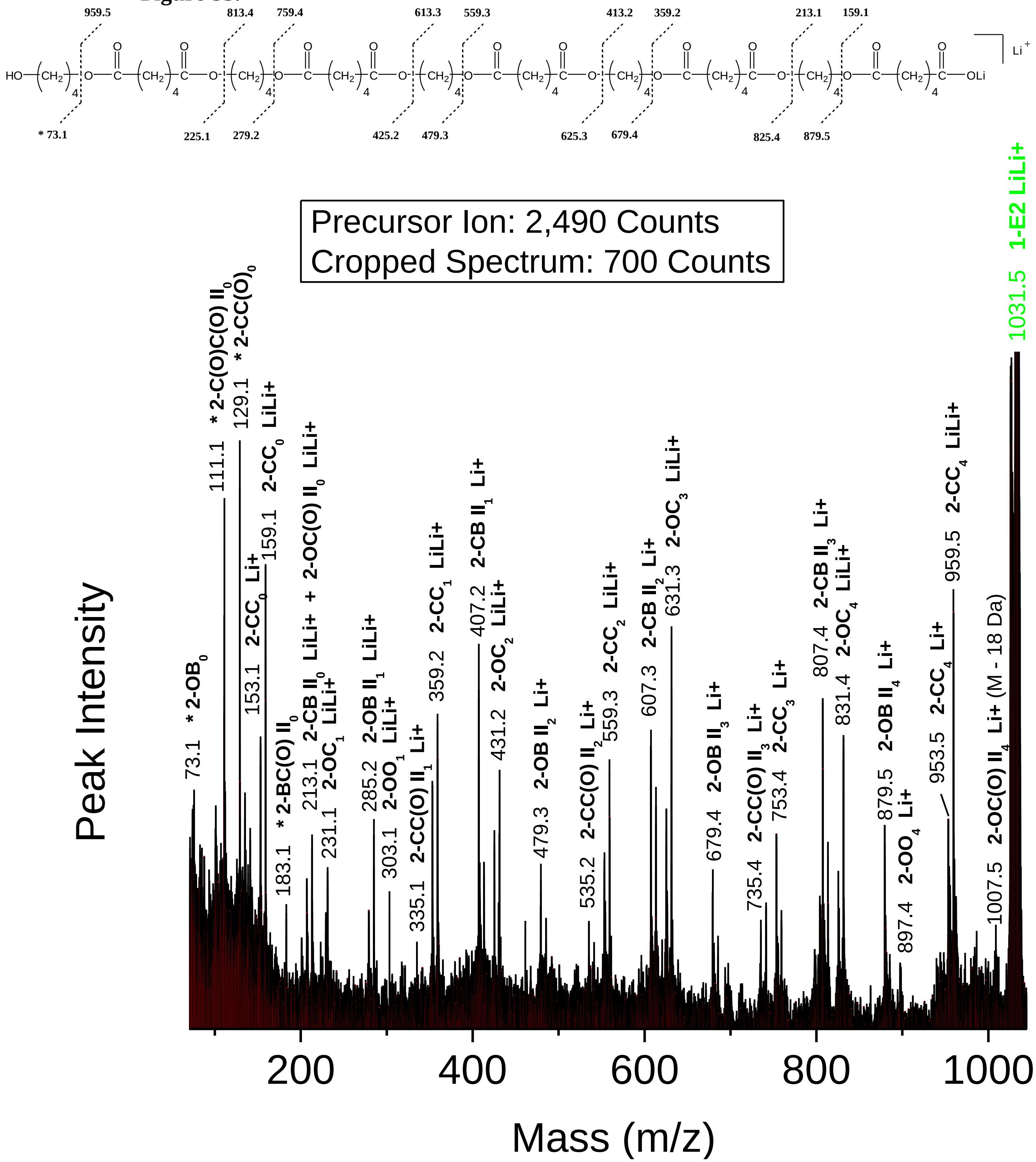
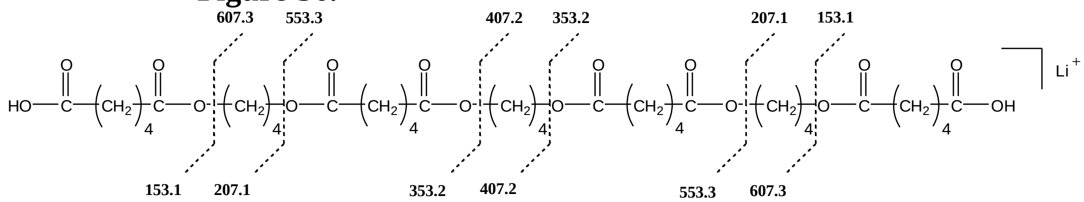

Precursor Ion: 2,490 Counts
Cropped Spectrum: 700 Counts
Peak Intensity
Mass (m/z)
1031.5 1-E2 LiLi+

Figure S6.


607.3
553.3
407.2
353.2
207.1
153.1
Li+

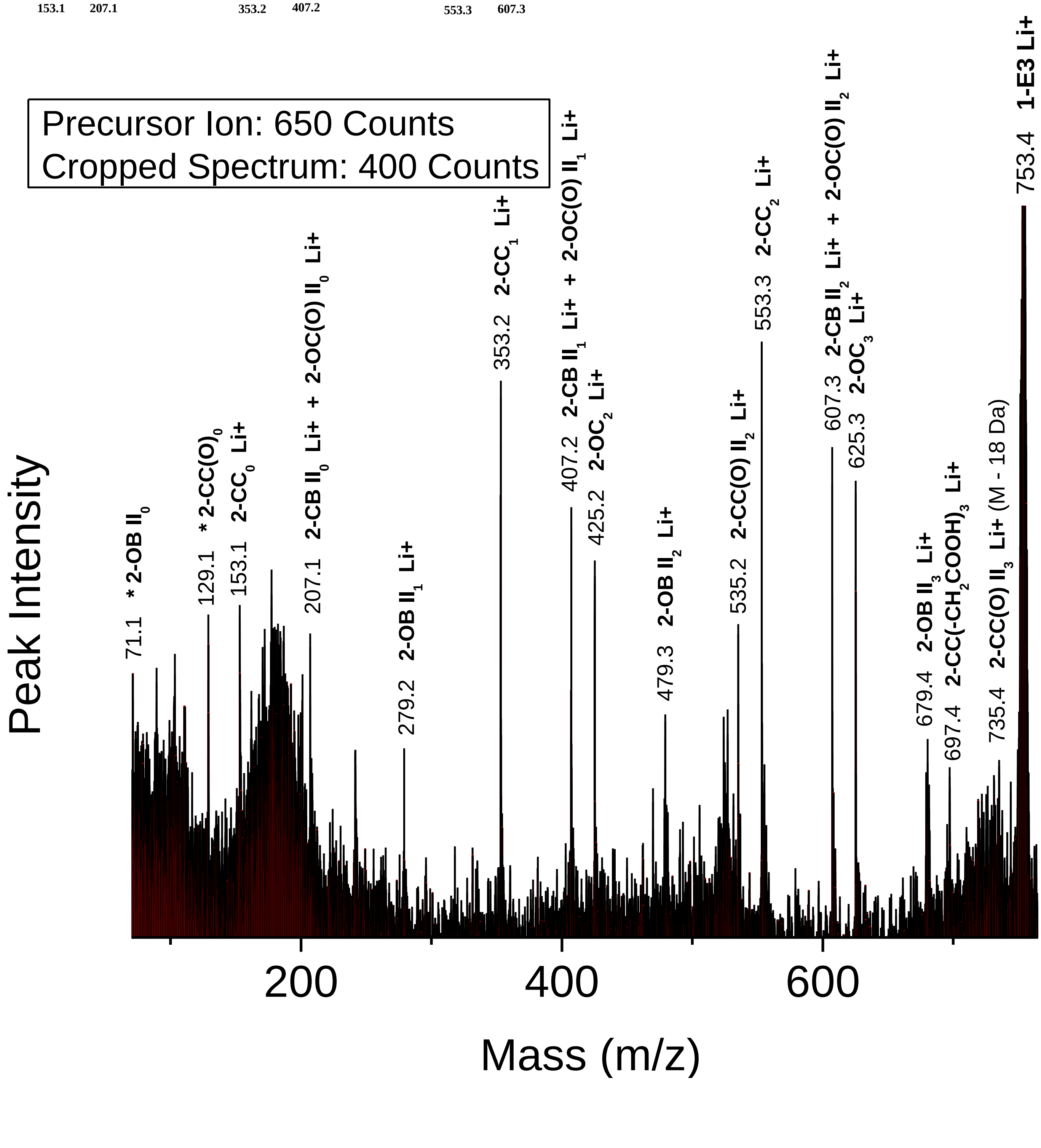
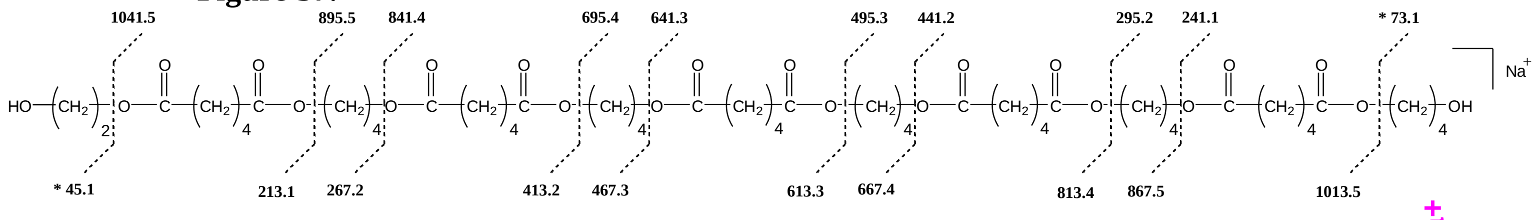
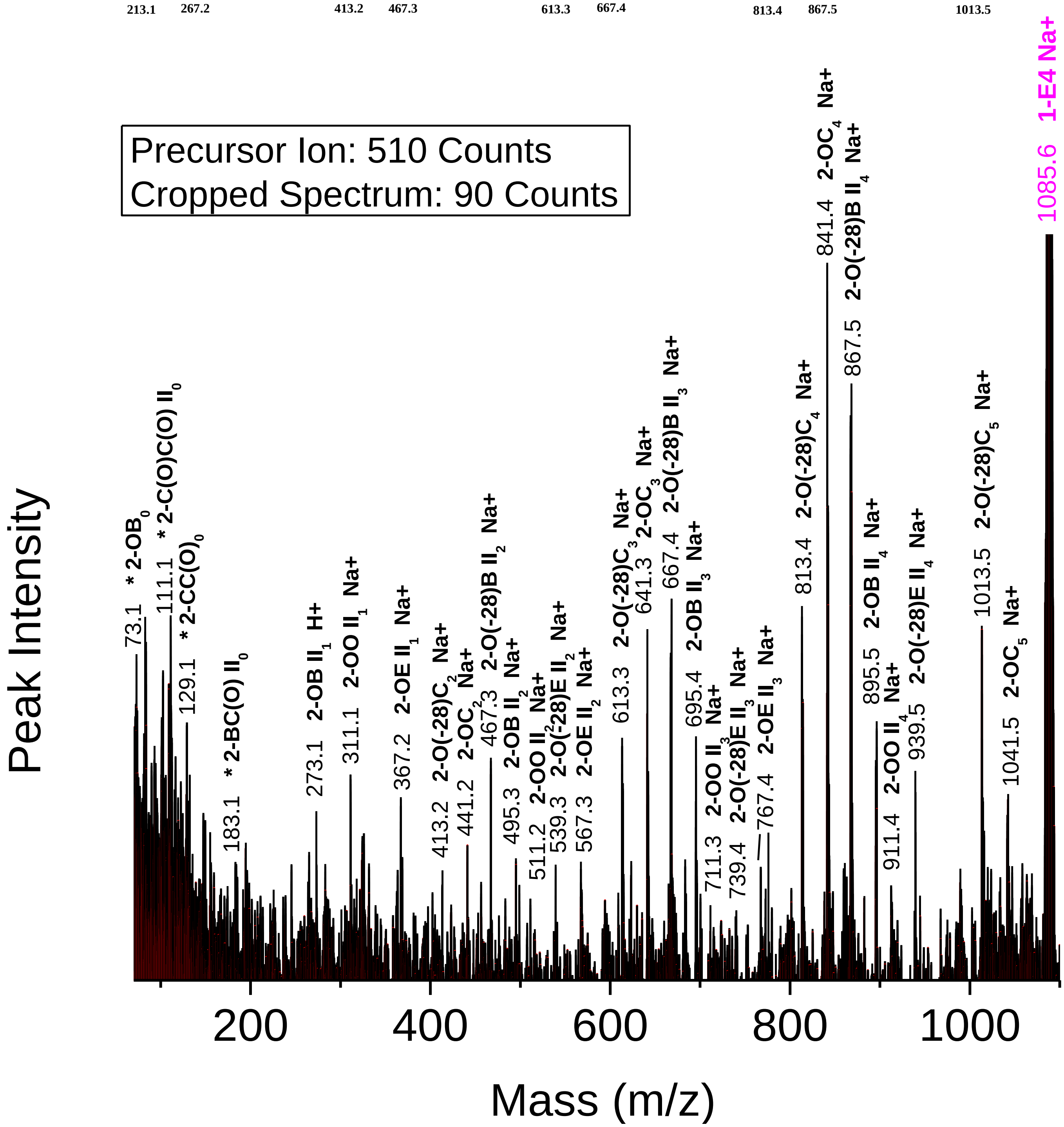

Precursor Ion: 650 Counts
Cropped Spectrum: 400 Counts
Peak Intensity
Mass (m/z)
200
400
600
71.1 * 2-OB II0
129.1 * 2-CC(O)0
153.1 2-CC0 Li+
207.1 2-CB II0 Li+ + 2-OC(O) II0 Li+
279.2 2-OB II1 Li+
353.2 2-CC1 Li+
407.2 2-CB II1 Li+ + 2-OC(O) II1 Li+
425.2 2-OC2 Li+
479.3 2-OB II2 Li+
535.2 2-CC(O) II2 Li+
553.3 2-CC2 Li+
607.3 2-CB II2 Li+ + 2-OC(O) II2 Li+
625.3 2-OC3 Li+
679.4 2-OB II3 Li+
697.4 2-CC(-CH2COOH)3 Li+
735.4 2-CC(O) II3 Li+ (M - 18 Da)
753.4 1-E3 Li+

Figure S7.


1041.5
895.5
841.4
695.4
641.3
495.3
441.2
295.2
241.1
* 73.1
* 45.1
213.1
267.2
413.2
467.3
613.3
667.4
813.4
867.5
1013.5
Na+


Precursor Ion: 510 Counts
Cropped Spectrum: 90 Counts
Peak Intensity
Mass (m/z)
1085.6 1-E4 Na+
841.4 2-OC4 Na+
867.5 2-O(-28)B II4 Na+
813.4 2-O(-28)C4 Na+
1013.5 2-O(-28)C5 Na+
1041.5 2-OC5 Na+
667.4 2-O(-28)B II3 Na+
641.3 2-OC3 Na+
613.3 2-O(-28)C3 Na+
73.1 * 2-OB0
111.1 * 2-C(O)C(O) II0
129.1 * 2-CC(O)0
183.1 * 2-BC(O) II0
273.1 2-OB II1 H+
311.1 2-OO II1 Na+
367.2 2-OE II1 Na+
413.2 2-O(-28)C2 Na+
441.2 2-OC2 Na+
467.3 2-O(-28)B II2 Na+
495.3 2-OB II2 Na+
511.2 2-OO II2 Na+
539.3 2-O(-28)E II2 Na+
567.3 2-OE II2 Na+
695.4 2-OB II3 Na+
711.3 2-OO II3 Na+
739.4 2-O(-28)E II3 Na+
767.4 2-OE II3 Na+
895.5 2-OB II4 Na+
911.4 2-OO II4 Na+
939.5 2-O(-28)E II4 Na+
200
400
600
800
1000