Supporting Information

Detailed Glycan Structural Characterization by Electronic Excitation Dissociation*

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Supporting Information

Table of Contents

Methods

Materials

Sialyl lewis A (SLe^A), sialyl lewis X (SLe^X), lacto-*N*-tetraose (LNT), and lacto-*N*-neotetraose (LNnT) were purchased from Dextra Laboratories (Reading, UK). Maltoheptaose, dextran ladder, ribonuclease B (RNase B), $H_2{}^{18}O$ (97%) water, 2-aminopyridine, acetic acid, and reagents for permethylation including dimethyl sulfoxide (DMSO), sodium hydroxide (NaOH), methyl iodide (CH_3I), and chloroform, as well as all salts including lithium acetate, sodium acetate, sodium borohydride ($NaBH_4$), potassium acetate, cesium acetate were obtained from Sigma-Aldrich (St. Louis, MO). Glycerol-free PNGase F was obtained from Prozyme (Hayward, CA). Sep-Pak™ C18 SPE cartridges were obtained from Waters (Milford, MA). Porous-graphitized carbon (PGC) solid phase extraction (SPE) columns were obtained from Thermo-Scientific (Springfield, NJ). Reversed-phase C18 ZipTips were obtained from Millipore (Billerica, MA). Microspin cellulose cartridges were purchased from Harvard Apparatus (Holliston, MA).

Reducing End Reduction

Reducing end reduction was performed on maltoheptaose according to the method reported by Costello *et al*.[1] Dried maltoheptaose (~100 µg) was dissolved in 200 µL of 0.1M NaOH / 1M $NaBH_4$ for 1 h at ambient temperature. Acetic acid (10%) was then added drop by drop until bubbling ceased. PGC SPE cartridges were used for desalting of the reduction product. PGC cartridges were pre-wetted with 100% acetonitrile followed by sequential rinses with 2 mL of 60%, 30%, and 0% acetonitrile/water, each containing 0.1% trifluoroacetic acid (TFA). The reduction product was loaded to a PGC cartridge, washed extensively with 0.1% TFA and eluted by 3 mL of 30% acetonitrile (ACN) in 0.1% TFA. The desalted and reduced maltoheptaose was then dried in a SpeedVac™ concentrator prior to permethylation.

Reducing End ^{18}O-Labeling

The reducing end ^{18}O-isotope labeling was performed based on the method introduced by Viseux *et al*.[2] The catalyst solution was prepared by dissolving 2.7 mg of 2-aminopyridine in 1.0 mL of anhydrous methanol. Dried native glycan (≤50 µg) was dissolved in 25 µL of $H_2^{18}O$ (97%) with 2.5 µL of the catalyst solution and 1 µL of acetic acid. The solution was then incubated at 37 °C overnight. After completion of the reaction, the ^{18}O-labeled glycans were dried in a SpeedVac™ concentrator prior to permethylation.

Reducing End 2-AB Labeling

The reducing end 2-AB labeling was performed as described previously.[3] Briefly, the labeling reagent solution was prepared by dissolving 6 mg of dried 2-aminobenzamide (2-AB) and 6 mg of dried sodium cyanoborohydride ($NaBH_3CN$) in 100 µL of acetic acid:DMSO (3:7, *v*:*v*) solution. The oligosaccharide (10 µg) was dissolved in 10 µL of the reagent solution and was incubated at 65 ºC for 3 h. Excess reagents were then removed with microspin cellulose cartridges (Harvard Apparatus, Holliston, MA).

N-linked Glycan Release from Ribonuclease B

The high-mannose *N*-linked glycans were released from RNase B by PNGase F according to the Glyko® *N*-Glycanase protocol by Prozyme. Dried glycoprotein (500 µg) was dissolved in 45 µL of 1X Tris reaction buffer and 2.5 µL of denaturation solution. The glycoprotein was then denatured in boiling water for 5 min. After denaturation, 2.5 µL of detergent solution and 2 µL of PNGase F were added. The mixture of glycoprotein and PNGase F was incubated at 37 °C overnight. Sep-Pak™ C18 SPE cartridges were used to separate the released *N*-linked glycans from the protein. The C18 SPE cartridge was sequentially rinsed with 10 mL of 100% ACN, 50% ACN, and water. The mixture containing high mannose *N*-linked glycan, deglycosylated ribonuclease B and PNGase F was then loaded to the cartridge. The *N*-linked glycans were eluted from the cartridge with 3 x 2 mL water. The purified *N*-linked glycans were then dried in a SpeedVac™ concentrator.

Permethylation

Permethylation was performed using the method introduced by Ciucanu and Kerek[4] and modified by Ciucanu and Costello.[5] The native glycan was suspended in 100 μL of DMSO/NaOH solution and was left at room temperature for 1 h, with vortexing every 15 min. CH_3I (50 μL) was then added to the reaction mixture and the reaction was allowed to proceed for another 1 h, with vortexing every 15 min. Additional NaOH/DMSO (100 μL) and CH_3I (50 μL) were then added together, and the reaction was allowed to proceed for at least 1 h longer, with vortexing every 15 min. After the completion of the reaction, 300 μL of chloroform was added to stop the permethylation reaction and to extract the permethylated glycans. Water (400 μL) was added to wash out the salts in the sample. The sample tubes were vortexed and centrifuged. The upper aqueous layer was removed and the organic phase was retained. The washing cycle was repeated at least 5 times.

Electrospray Conditions

Permethylated oligosaccharides were dissolved in 25% methanol, 20-250 μM salt solutions to a concentration of 5 μM for electrospray ionization (ESI) tandem MS analysis. Samples were loaded into a glass capillary tip pulled with a micropipette puller (model P-97; Sutter Instruments Co., Novato, CA) to ~1 μm orifice diameter. A bare nickel chromium wire was inserted into the sample solution on the distal end of the tip to form the electrical connection. Samples were then directly infused into the mass spectrometer ion source.

Tandem Mass Spectrometry

The tandem mass spectrometry (MS/MS) experiments were performed on a 12-T solariX™ hybrid Qq-FTICR mass spectrometer equipped with an indirectly heated hollow dispenser cathode (Bruker Daltonics, Bremen, Germany). Target ions were isolated by a front-end quadrupole and accumulated in the collision cell for 100 to 500 ms before being transferred to the ICR cell. For low-energy ECD, the precursor ions were irradiated with ~1.5 eV electrons for 100 ms; for EED, the precursor ions were irradiated with 14 eV electrons, for 0.2 to 0.5 s. The cathode heating current was from 1.32 A to 1.52 A. A 0.5 s transient was typically acquired. Each ExD spectrum shown is the result of multiple transients summed to improve the signal-to-noise ratio.

On-line LC-MS/MS Analysis

On-line reversed phase liquid chromatographic separation was carried out on a nanoACQUITY UPLC system (Waters, Milford, MA). Ten ng of reduced and permethylated maltodextrin was loaded onto a self-packed capillary trapping column (150 μm x 30 mm, C18, 5 μm particle size, 200 Å) and separated by an analytical column (150 μm x 100 mm, C18, 3 μm particle size, 100 Å) at 35 ^{o}C. The solvent system consisted of 0.1% formic acid in 1% acetonitrile (solvent A) and 0.1% formic acid in 99% acetonitrile (solvent B). The gradient program included a 4-min trapping at a flow rate of 4 μL/min in 80% solvent A and 20% solvent B, followed by separation at a flow rate of 500 nL/min, using a 20-80% linear gradient of solvent B over 40 min. At the end of the separation, the gradient was ramped to 99% of solvent B over 2 min and stayed for 3 min, before returning to 20% of solvent B in 2 min, followed by equilibration to the original condition for 12 min.

LC-eluent was infused into the solariX mass spectrometer using a nanoESI source. The instrument was externally calibrated using sodium trifluoroacetate ion clusters over the range *m/z* 200 - 3000 with 1 M data points, giving a transient length of 0.58 s and an FT-limited mass resolving power of 130,000 at *m/z* 400. For LC-MS/MS experiments, data-dependent acquisition was performed with the system switching between the MS and MS/MS modes. 0.2-s ion accumulation was used for each MS scan, and 2.5-s ion accumulation was used for each MS/MS scan. Preferred and exclusion lists were used to select ions of interest for tandem MS analysis. The precursor ions were isolated in the quadrupole with an isolation window of 6 *m/z*. For EED experiments, the electron irradiation time was 0.5 s, with the cathode heating currents set at 1.52 A, the cathode bias potential at -15 V, and the extraction lens voltage set at -15.05 V.

Data Analysis

All spectra were zero-filled twice and Fourier transformed without apodization. The MS/MS spectra were internally calibrated using a few fragment ions assigned with high confidence, giving a typical mass measurement accuracy of 2 ppm or better. Deconvoluted mass lists were generated semi-automatically by the SNAP™ (Sophisticated Numerical Annotation Procedure) algorithm[6] using the DataAnalysis™ software (Bruker Daltonics) and verified manually. Software used to assist in data analysis include GlycoWorkBench,[7] and a home-made Visual Basic program for auto-assignment. The nomenclature used for designating carbohydrate fragments was that introduced by Domon and Costello.[8]

References

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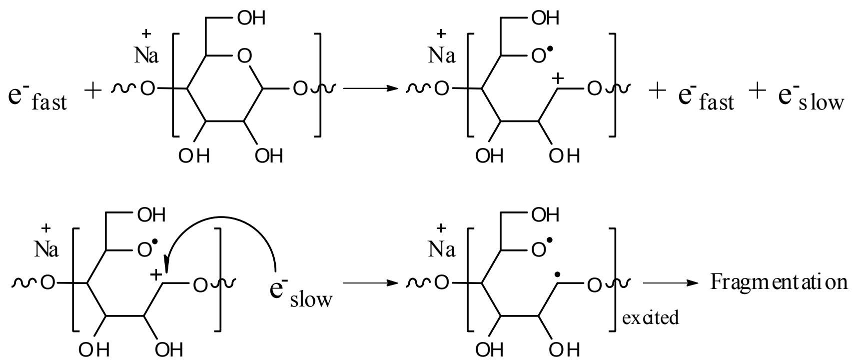
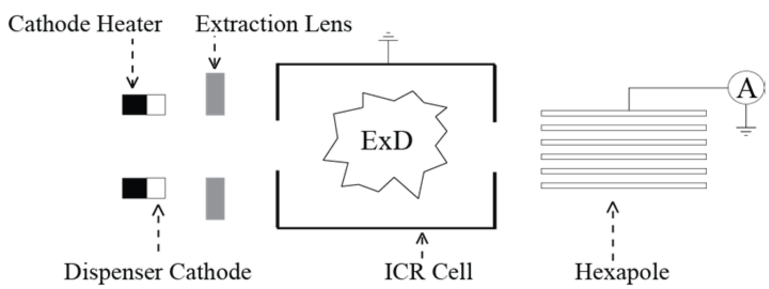
[7] a) A. Ceroni, A. Dell, S. M. Haslam, *Source Code for Biology and Medicine* **2007**, *2*, 3; b) A. Ceroni, K. Maass, H. Geyer, R. Geyer, A. Dell, S. M. Haslam, *J. Proteome. Res.* **2008**, *7*, 1650-1659.
[8] B. Domon, C. E. Costello, *Glycoconjugate J.* **1988**, *5*, 397-409.

Supplemental Schemes



Scheme S1. EED is initiated by electron detachment from an oxygen atom, forming a distonic ion (top). The subsequent electron re-capture produces a di-radical which then undergoes extensive fragmentation (bottom).



Scheme S2. Schematics of the ExD experimental setup.

Supplemental Figures

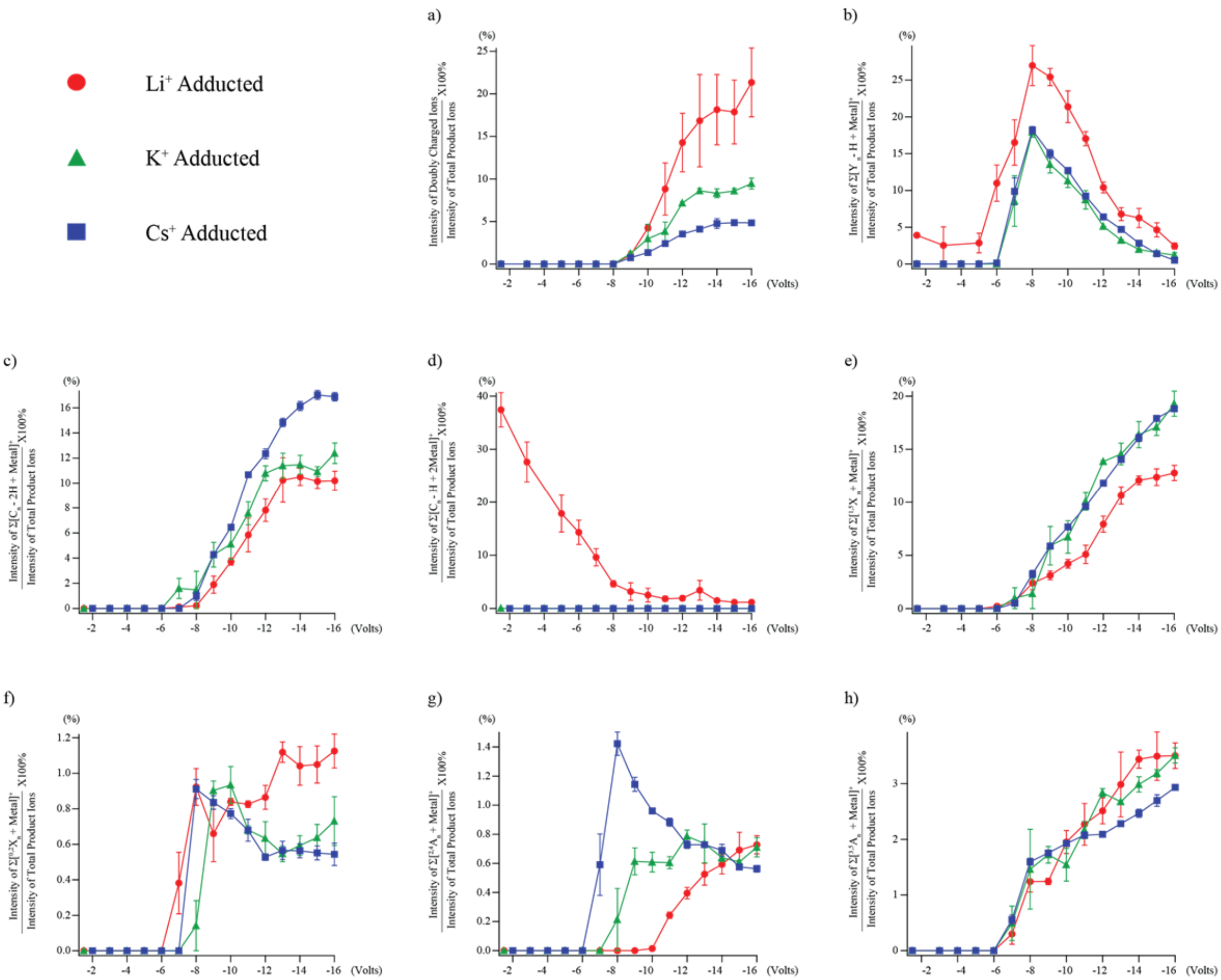


Figure S1. The ExD fragmentation pattern of metal-adducted glycans is affected by both the electron energy and the charge carrier. Reduced and permethylated maltoheptaose was selected as the model glycan. With 1.32 A cathode heating current, precursor ions adducted with either two Li^+ (red circle, *m/z* 752.4013), two K^+ (green triangle, *m/z* 784.3490), or two Cs^+ (blue square, *m/z* 878.2907) were isolated and irradiated with electrons at different energies, ramping from 1 eV to 16 eV at 1-eV intervals. The x axis represents the voltage applied to the cathode dispenser. The y axis represents the percentage ratio of the intensity of a specific type of fragment ion and the total product ion intensity. Fragment ions plotted are a) doubly charged ions, b) $[Y - H + 2Metal]^+$ ions, c) $[C - 2H + Metal]^+$ ions, d) $[C - H + 2Metal]^+$ ions, e) $[^{1,5}X + Metal]^+$ ions, f) $[^{0,2}X + Metal]^+$ ions, g) $[^{2,4}A + Metal]^+$ ions, and h) $[^{3,5}A + Metal]^+$ ions, respectively. The relative abundance of linkage definitive cross-ring fragments increased significantly as the electron energy approached the EED region.

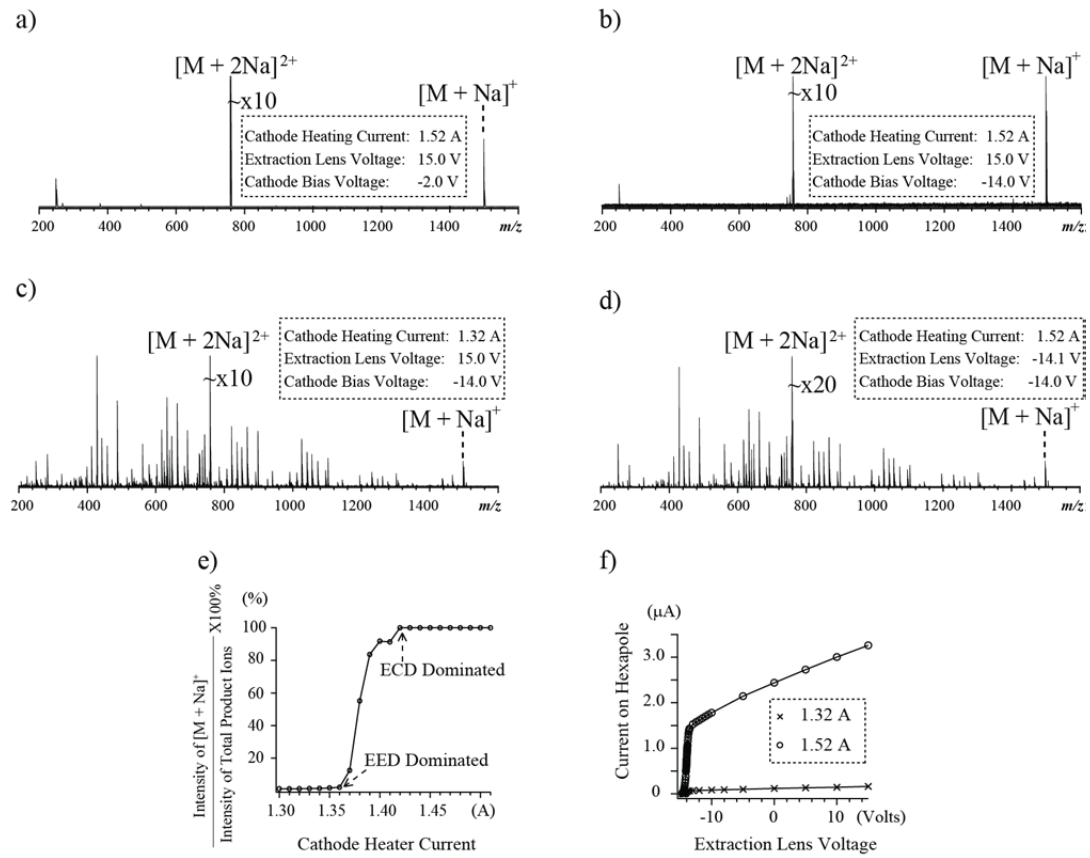


Figure S2. Influence of the cathode heating current and the extraction lens voltage on the fragmentation pattern of the doubly sodiated permethylated maltoheptaose ($[M + 2Na]^{2+}$, *m/z* 760.3594). a) With a cathode heating current of 1.52 A, an ECD experiment can be carried out by setting the cathode bias to -2.0 V and the extraction lens voltage to 15.0 V. b) The ECD process still dominated even when the kinetic energy of electrons was elevated to 14.0 eV by decreasing the cathode bias from -2 V to -14 V. Efficient EED can be obtained either c) by lowering the cathode heating current to 1.32 A or d) by setting the extraction lens voltage (-14.1 V) close to the cathode bias (-14.0 V). e) The ECD efficiency dropped exponentially with the decreasing cathode heating current. The ratio of the abundance of the charge reduced species, $[M + Na]^+$, to the total product ion abundance was used as an indicator for the ECD efficiency. f) With the cathode bias set to -14.0 V, the electron current measured at the hexapole decreased as the extraction lens voltage decreased.

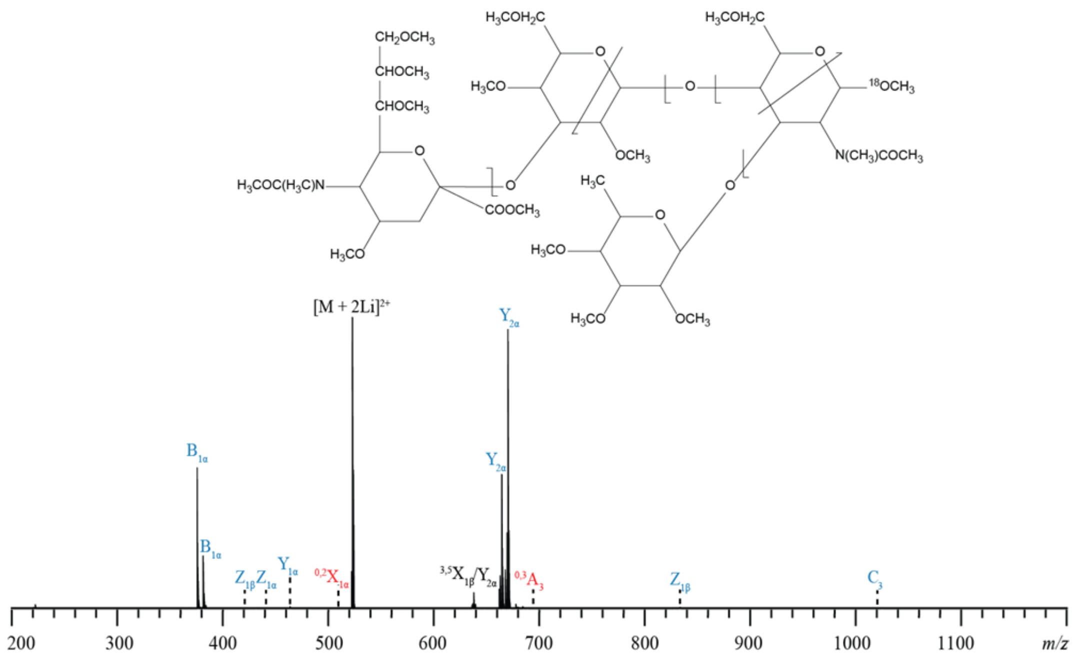


Figure S3. The CID cleavage map and the CID spectrum of the doubly lithiated, permethylated and ^{18}O-labeled SLe^{X} precursor ion at *m/z* 523.2830. The detailed product ion list can be found in Table S2.

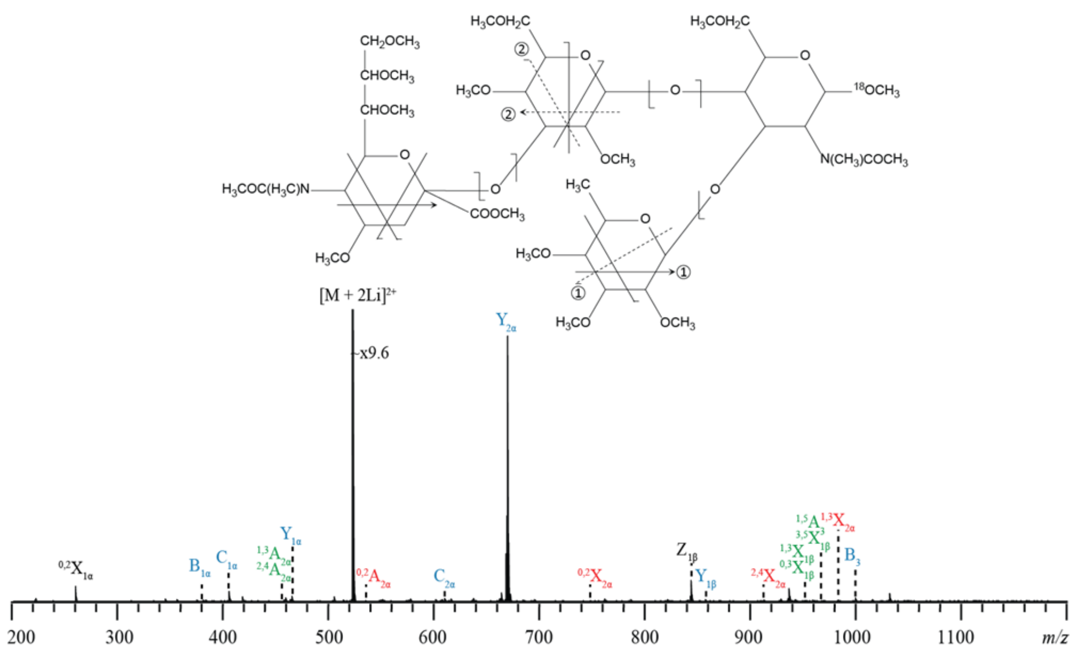


Figure S4. The ECD cleavage map and the ECD spectrum of the doubly lithiated, permethylated and ^{18}O-labeled SLe^{X} precursor ion at *m/z* 523.2830. The detailed product ion list can be found in Table S3.

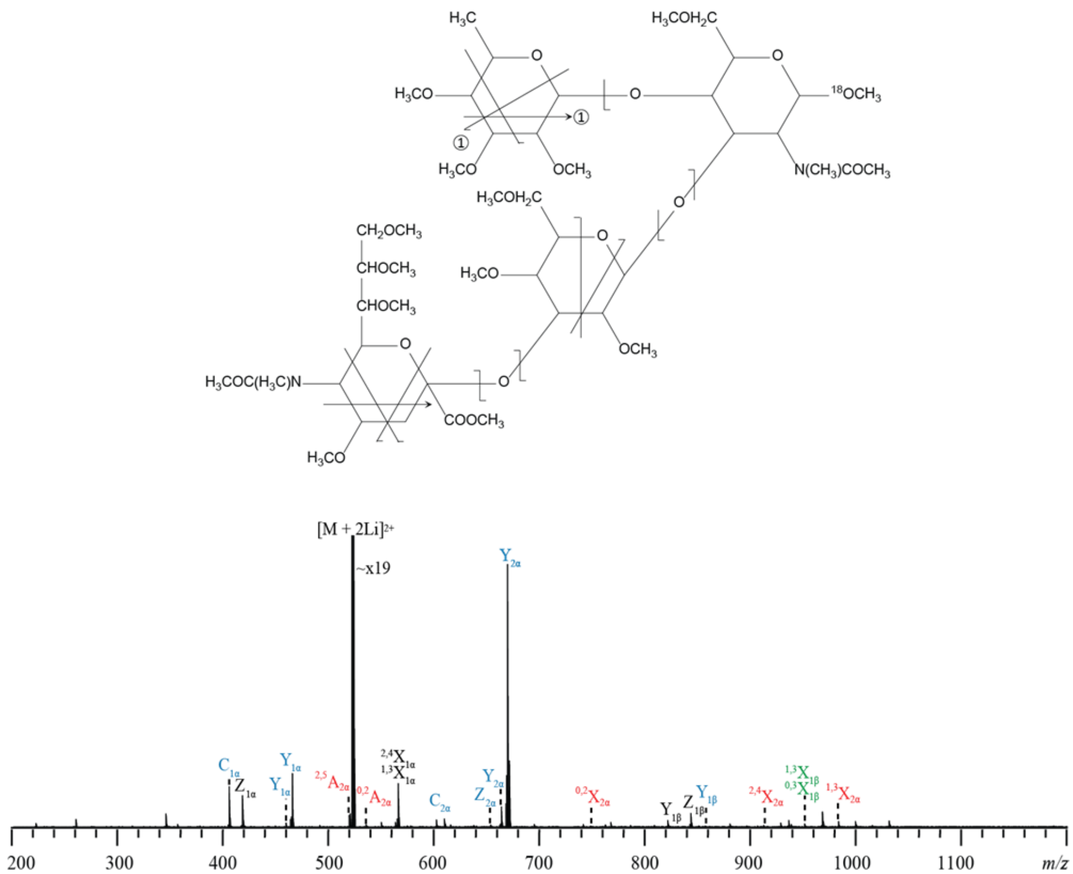


Figure S5. The ECD cleavage map and the ECD spectrum of the doubly lithiated, permethylated and ^{18}O-labeled SLe^{A} precursor ion at *m/z* 523.2830. The detailed product ion list can be found in Table S5.

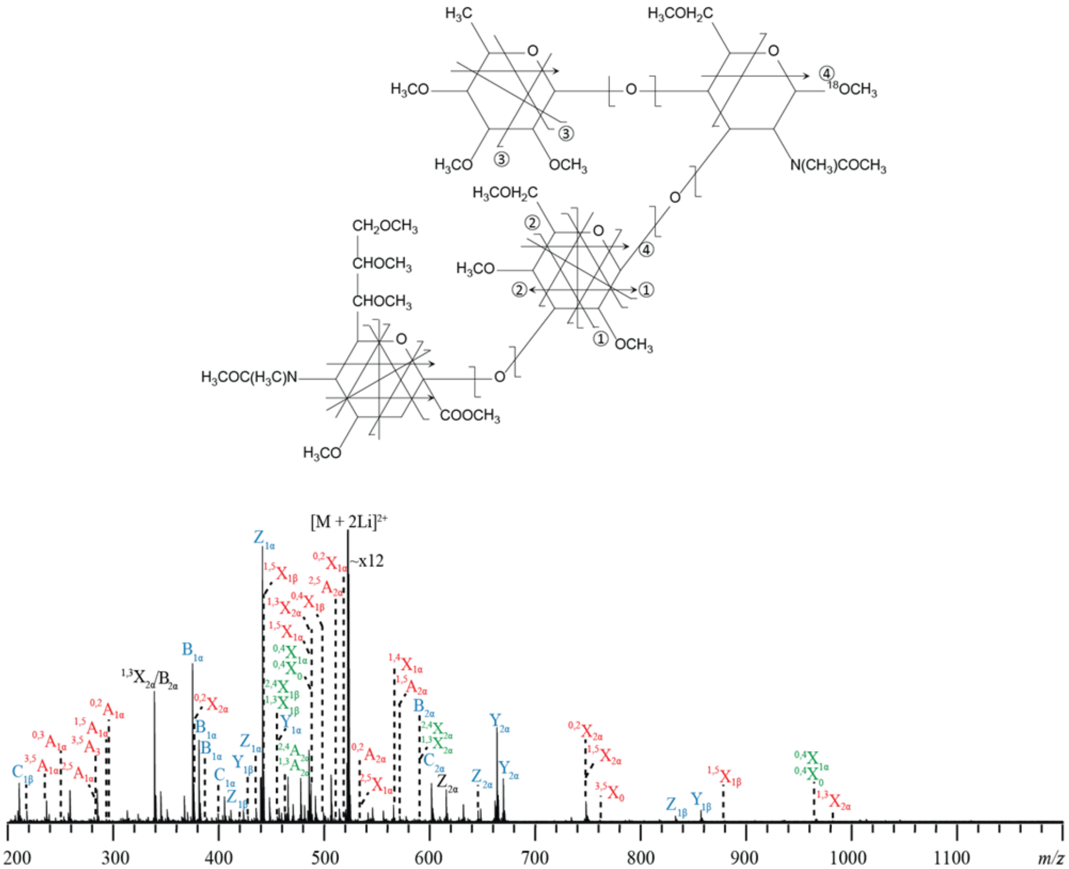


Figure S6. The EED cleavage map and the EED spectrum of the doubly lithiated, permethylated and ^{18}O-labeled SLe^{A} precursor ion at *m/z* 523.2830. The detailed product ion list can be found in Table S6.

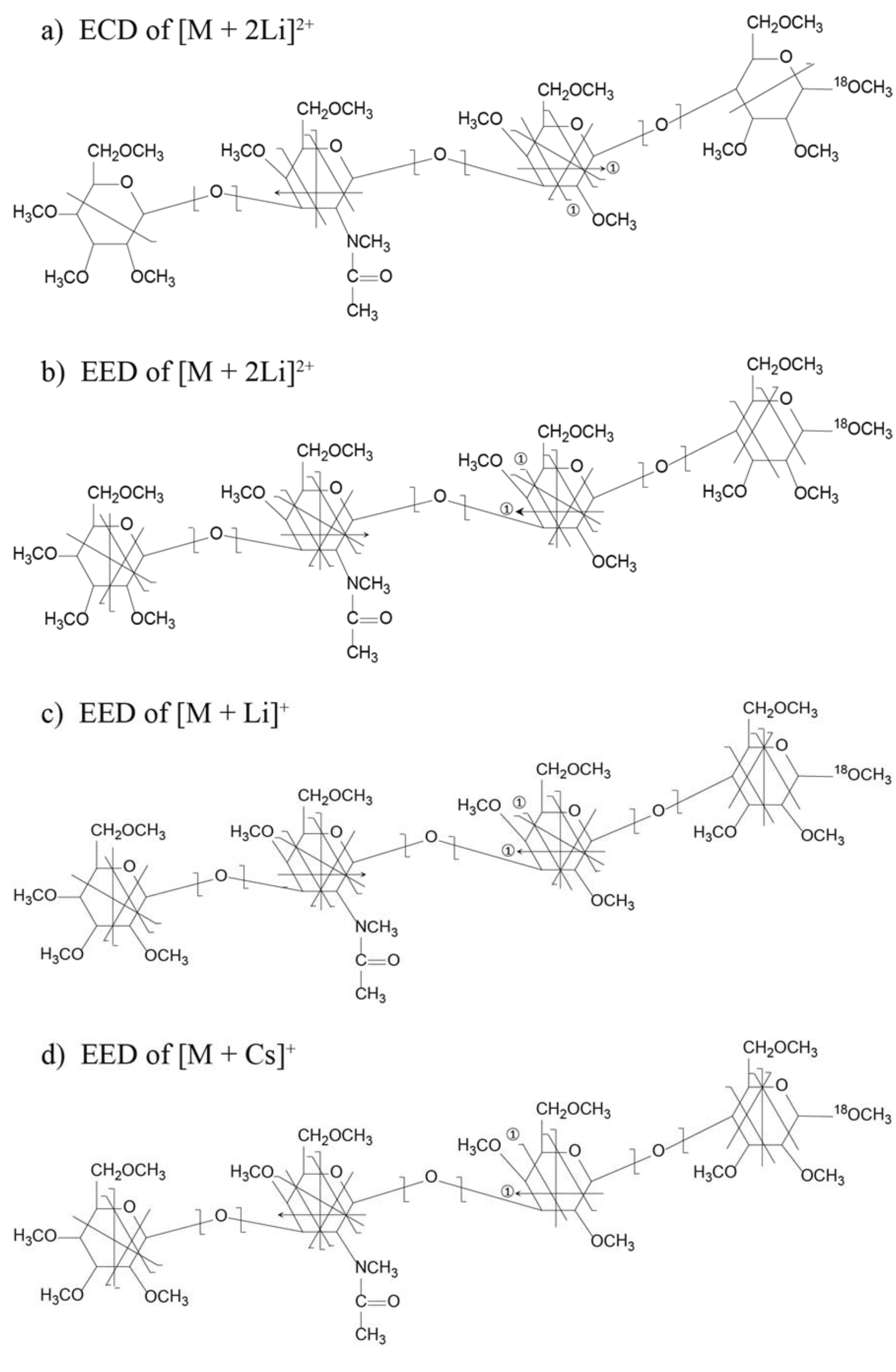


Figure S7. a) The ECD and b) EED cleavage maps of the doubly lithiated, permethylated, ^{18}O-labeled LNT at *m/z* 459.7513; c) the EED cleavage map of the singly lithiated, permethylated, ^{18}O-labeled LNT at *m/z* 912.4872; d) the EED cleavage map of the singly cesiated, permethylated, ^{18}O-labeled LNT at *m/z* 1038.3767. The detailed product ion lists can be found in Tables S7 to S10.

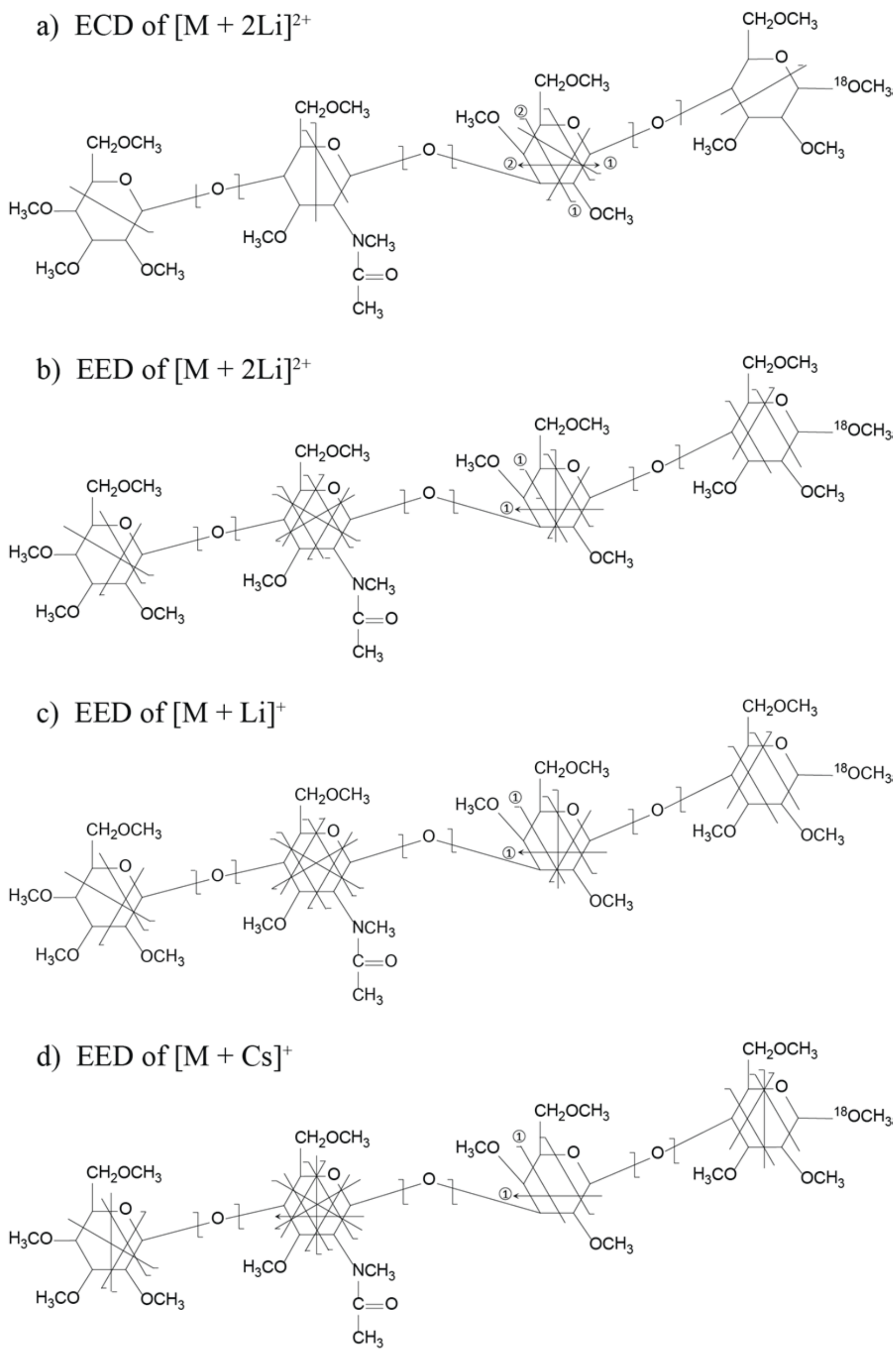


Figure S8. a) The ECD and b) EED cleavage maps of the doubly lithiated, permethylated, ^{18}O-labeled LNnT at *m/z* 459.7513; c) the EED cleavage map of the singly lithiated, permethylated, ^{18}O-labeled LNnT at *m/z* 912.4872; d) the EED cleavage map of singly cesiated, permethylated, ^{18}O-labeled LNnT at *m/z* 1038.3767. The detailed product ion list can be found in Table S11 to S14.

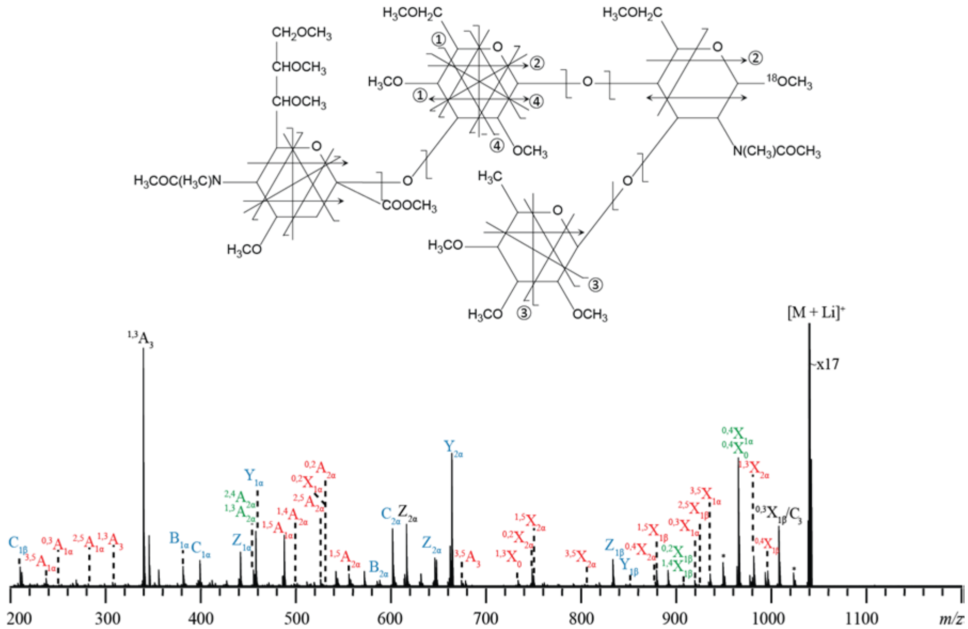


Figure S9. The EED cleavage map and spectrum of the singly lithiated, permethylated and ^{18}O-labeled SLe^{X} precursor ion at *m/z* 1039.5505. The detailed product ion list can be found in Table S15.

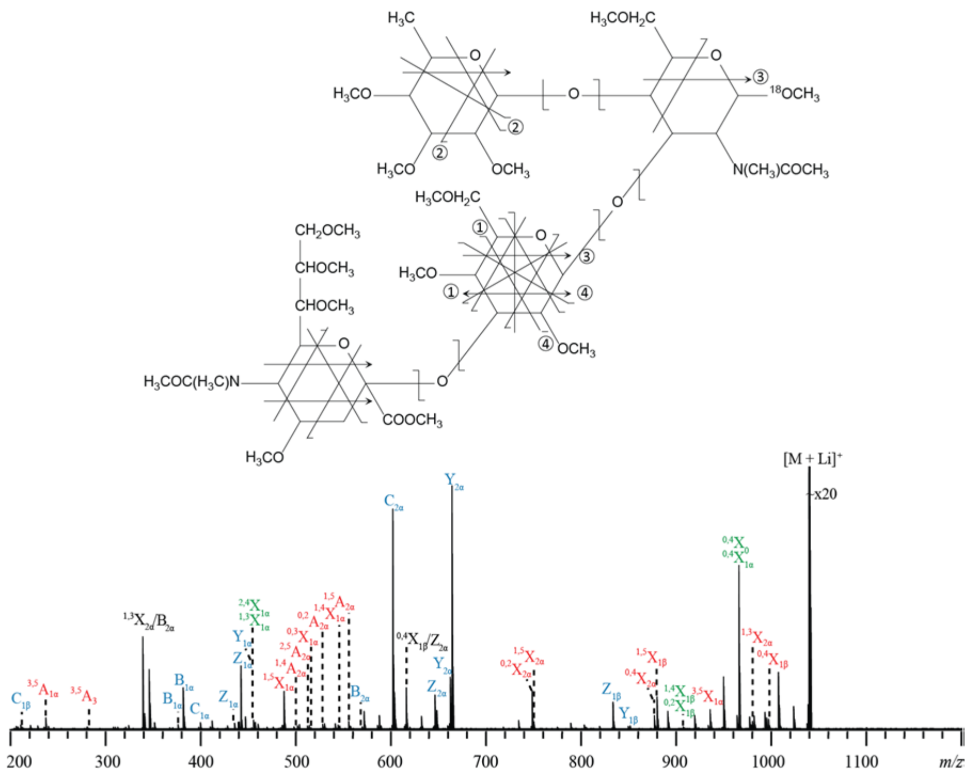


Figure S10. The EED cleavage map and spectrum of the singly lithiated, permethylated and ^{18}O-labeled SLe^{A} precursor ion at *m/z* 1039.5505. The detailed product ion list can be found in Table S16.

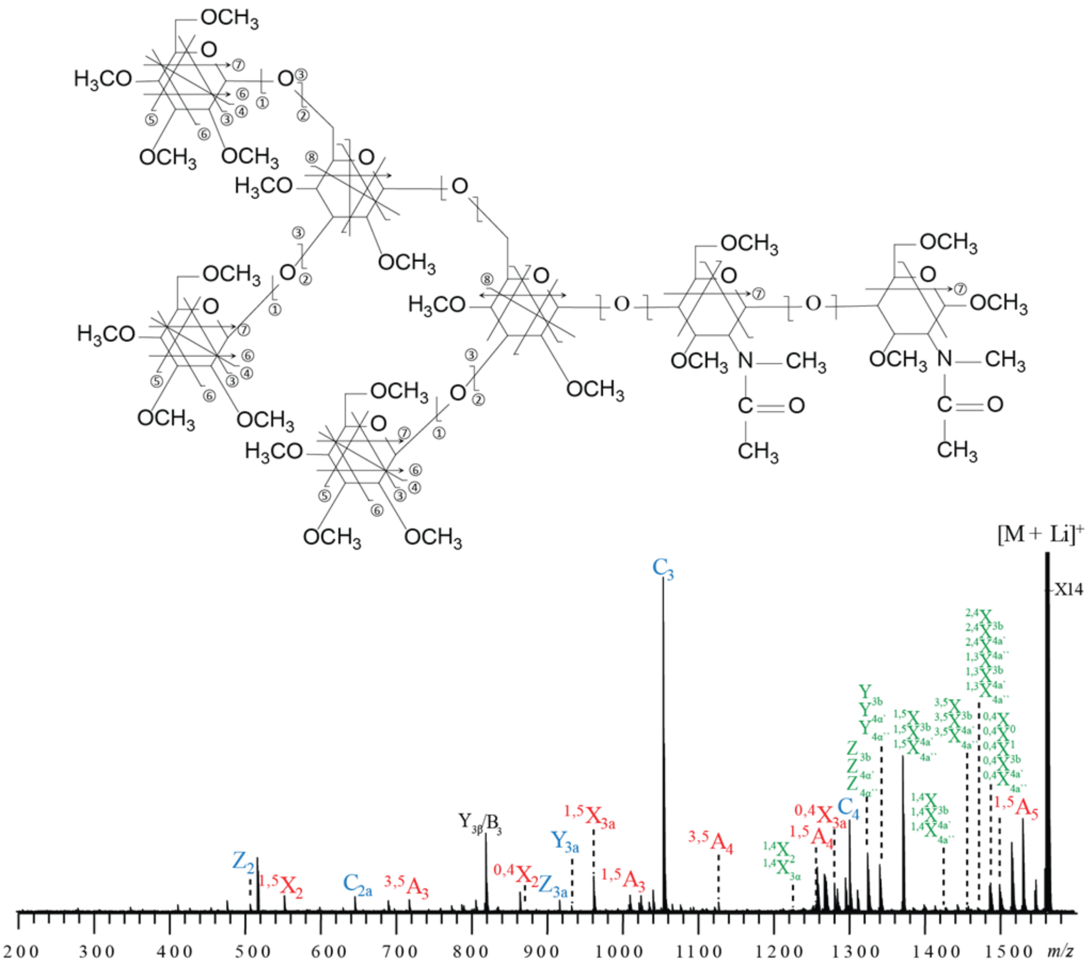


Figure S11. The EED cleavage map and spectrum of the singly lithiated and permethylated $(Man)_5(GlcNAc)_2$ at *m/z* 1563.8808. The detailed product ion list can be found in Table S17.

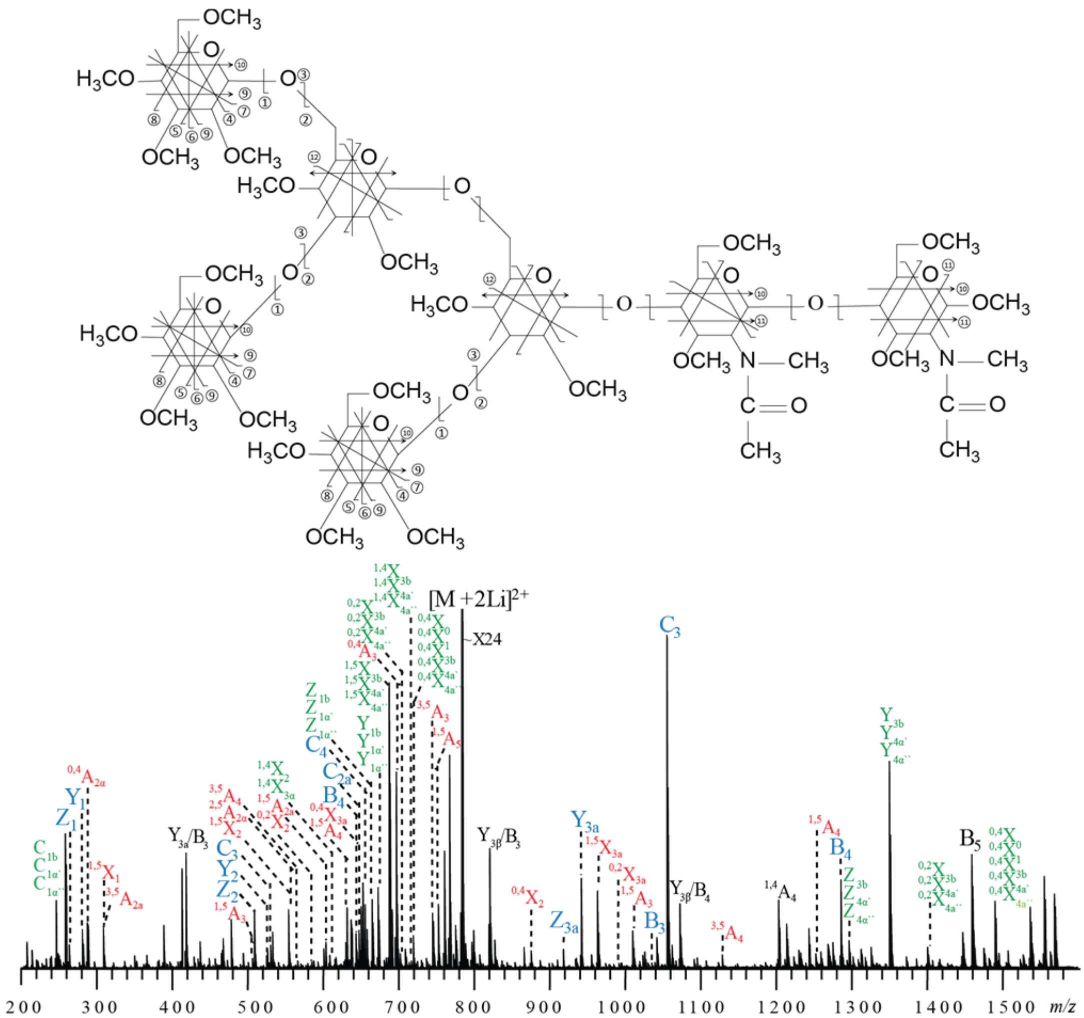


Figure S12. The EED cleavage map and spectrum of the doubly lithiated and permethylated $(Man)_5(GlcNAc)_2$ at *m/z* 785.4121. The detailed product ion list can be found in Table S18.

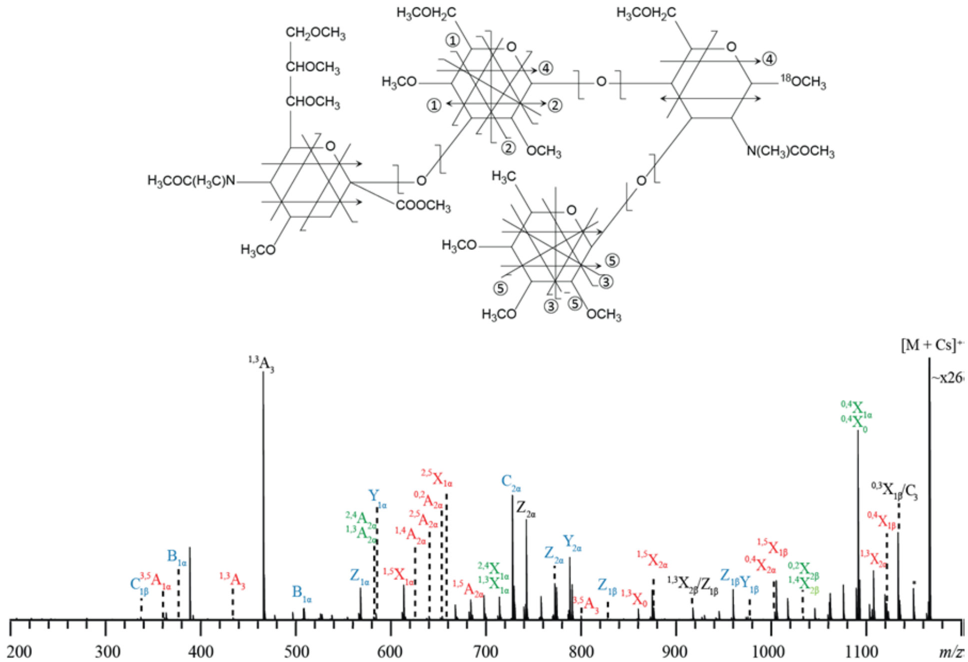


Figure S13. The EED cleavage map and spectrum of the singly cesiated, permethylated, ^{18}O-labeled SLe^{X} at *m/z* 1165.4400. The detailed product ion list can be found in Table S19.

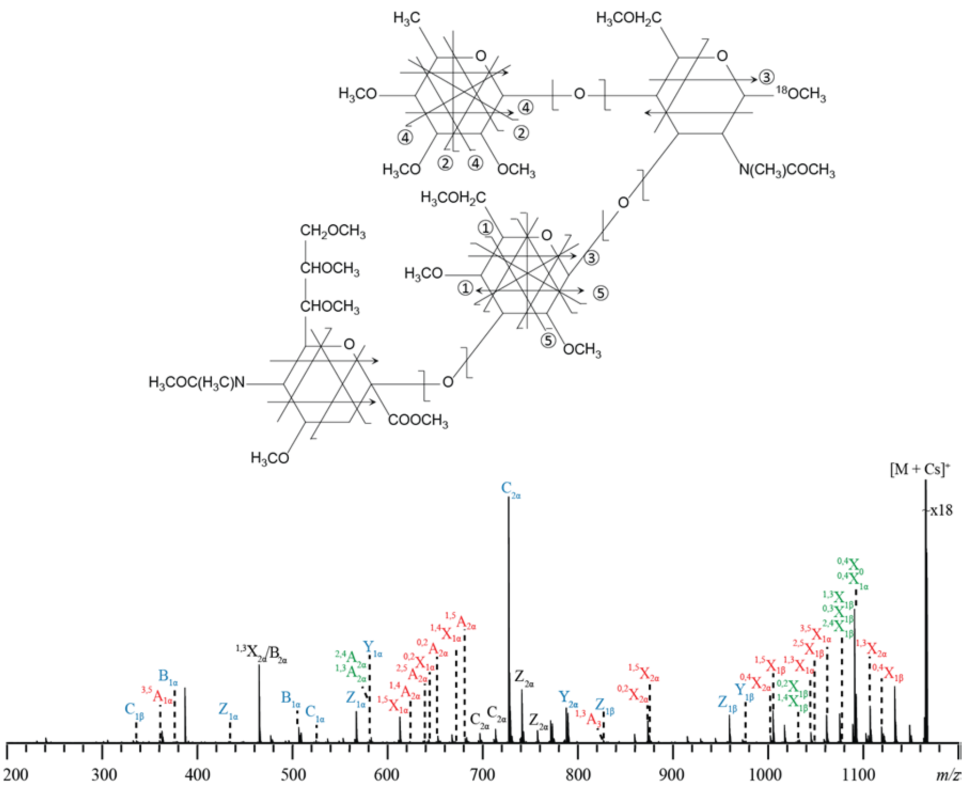


Figure S14. The EED cleavage map and spectrum of the singly cesiated, permethylated, ^{18}O-labeled SLe^{A} at *m/z* 1165.4400. The detailed product ion list can be found in Table S20.

Supplemental Tables

Table S1. The electron current measured at the hexapole at two different cathode bias voltage settings. The extraction lens voltage was 15.0 V, and the cathode heating current was 1.52 A.

Cathode bias voltage (V)	-2	-14
Electron current measured at the hexapole (nA)	0.349	3260

Table S2. List of CID fragment ions of the doubly lithiated, permethylated, and ^{18}O-Labeled Sialyl Lewis X at *m/z* 523.2830.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass)	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
376.1967	51.83	1	376.1966	0.21	$B_{1\alpha}$	H	0
382.2048	19.42	1	382.2048	0.05	$B_{1\alpha}$		+1Li
420.2252	0.18	2	840.4511	-0.90	$Z_{1\beta}$		+2Li
442.2509	0.15	1	442.2509	-0.03	$Z_{1\alpha}$		+1Li
458.2455	0.10	1	458.2458	-0.64	$Y_{1\alpha}$	-2H	+1Li
466.2696	0.50	1	466.2696	-0.09	$Y_{1\alpha}$	-H	+2Li
507.2573	0.04	1	507.2560	2.52	$^{0,2}X_{1\alpha}$	-2H	0
514.2651	0.07	2	1028.5310	-0.83	C_3	-2H	+2Li
664.3611	47.59	1	664.3612	-0.20	$Y_{2\alpha}$		+1Li
670.3691	97.81	1	670.3694	-0.47	$Y_{2\alpha}$	-H	+2Li
692.3670	0.08	1	692.3676	-0.76	$^{0,3}A_3$	2H	+1Li
827.4268	0.20	1	827.4269	-0.16	$Z_{1\beta}$	H	0
833.4352	0.55	1	833.4351	0.06	$Z_{1\beta}$		+1Li
1023.5322	0.39	1	1023.5306	1.54	C_3		+1Li

Table S3. List of ECD fragment ions of the doubly lithiated, permethylated, and ^{18}O-Labeled Sialyl Lewis X at *m/z* 523.2830.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
261.6424	0.22	2	523.2873	-4.83	$^{0,2}X_{1\alpha}$	CH_2	0
376.1965	0.05	1	376.1966	-0.28	$B_{1\alpha}$	H	0
382.2048	0.05	1	382.2048	0.05	$B_{1\alpha}$		+1Li
384.2205	0.04	1	384.2204	0.14	$B_{1\alpha}$	2H	+1Li
390.2287	0.02	1	390.2286	0.22	$B_{1\alpha}$	H	+2Li
406.2235	0.44	1	406.2235	-0.03	$C_{1\alpha}$	-H	+2Li
458.2573	0.05	1	458.2572	0.19	$^{1,3}A_{2\alpha}$	2H	+1Li
458.2573	0.05	1	458.2572	0.19	$^{2,4}A_{2\alpha}$	2H	+1Li
460.2614	0.13	1	460.2614	-0.09	$Y_{1\alpha}$		+1Li
466.2696	0.22	1	466.2696	-0.09	$Y_{1\alpha}$	-H	+2Li
536.2859	0.01	1	536.2865	-1.16	$^{0,2}A_{2\alpha}$	-H	+2Li
602.2993	0.07	1	602.2995	-0.28	$C_{2\alpha}$	-2H	+1Li
610.3232	0.12	1	610.3233	-0.22	$C_{2\alpha}$	-H	+2Li
662.3462	0.07	1	662.3456	0.94	$Y_{2\alpha}$	-2H	+1Li
664.3612	0.35	1	664.3612	-0.02	$Y_{2\alpha}$		+1Li
670.3695	11.17	1	670.3694	0.17	$Y_{2\alpha}$	-H	+2Li
748.3826	0.02	1	748.3823	0.39	$^{0,2}X_{2\alpha}$		+1Li
843.4748	0.86	1	843.4746	0.22	$Z_{1\beta}$	3H	+2Li
851.4424	0.03	1	851.4457	-3.88	$Y_{1\beta}$		+1Li
857.4539	0.06	1	857.4539	0.06	$Y_{1\beta}$	-H	+2Li
912.4847	0.04	1	912.4872	-2.78	$^{2,4}X_{2\alpha}$	2H	+1Li
951.4968	0.03	1	951.4981	-1.36	$^{0,3}X_{1\beta}$		+1Li
951.4968	0.03	1	951.4981	-1.36	$^{1,3}X_{1\beta}$		+1Li
951.4968	0.03	1	951.4981	-1.36	$^{2,4}X_{1\beta}$		+1Li
969.5046	0.03	1	969.5013	3.35	$^{1,5}A_3$	-H	0
969.5046	0.03	1	969.5087	-4.26	$^{3,5}X_{1\beta}$	2H	+1Li
983.5224	0.05	1	983.5244	-1.96	$^{1,3}X_{2\alpha}$	2H	+1Li
999.5164	0.12	1	999.5119	4.51	B_3	H	0

Table S4. List of EED fragment ions of the doubly lithiated, permethylated, and ^{18}O-Labeled Sialyl Lewis X at *m/z* 523.2830.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
211.1152	1.20	1	211.1152	-0.15	$C_{1\beta}$	-2H	+1Li
213.1309	1.05	1	213.1309	0.09	$C_{1\beta}$		+1Li
219.1391	0.65	1	219.1391	0.16	$C_{1\beta}$	-H	+2Li
236.1468	0.23	1	236.1469	-0.27	$^{3,5}A_{1\alpha}$	-2H	+1Li
238.1625	0.39	1	238.1625	-0.05	$^{3,5}A_{1\alpha}$		+1Li
252.1418	0.18	1	252.1418	0.11	$^{0,3}A_{1\alpha}$	-2H	+1Li
280.1731	0.17	1	280.1731	0.05	$^{2,5}A_{1\alpha}$	-2H	+1Li
308.1679	0.14	1	308.1680	-0.25	$^{1,3}A_{3}$	-2H	+1Li
310.1838	0.13	1	310.1836	0.55	$^{1,3}A_{3}$		+1Li
311.1915	0.14	1	311.1915	0.12	$^{1,3}A_{3}$	H	+1Li
316.1919	0.08	1	316.1918	0.25	$^{1,3}A_{3}$	-H	+2Li
340.1942	5.93	1	340.1942	0.03	$^{1,3}A_{3}$	$+OCH_2$	+1Li
376.1966	5.31	1	376.1966	-0.03	$B_{1\alpha}$	H	0
382.2048	3.91	1	382.2048	0.05	$B_{1\alpha}$		+1Li
383.2126	0.97	1	383.2126	-0.06	$B_{1\alpha}$	H	+1Li
406.2235	0.79	1	406.2235	-0.03	$C_{1\alpha}$	-H	+2Li
420.2251	0.12	2	840.4511	-1.12	$Z_{1\beta}$		+2Li
436.2427	0.07	1	436.2427	-0.03	$Z_{1\alpha}$	H	0
442.2509	0.96	1	442.2509	-0.03	$Z_{1\alpha}$		+1Li
442.7270	0.11	2	885.4564	-2.76	$^{2,5}A_{3}$		0
443.2278	0.39	2	886.4566	-1.13	$^{1,5}X_{1\beta}$		+2Li
454.2259	0.08	1	454.2259	-0.04	$^{1,3}A_{2\alpha}$	-2H	+1Li
454.2259	0.08	1	454.2259	-0.04	$^{2,4}A_{2\alpha}$	-2H	+1Li
456.2416	0.46	1	456.2415	0.11	$^{1,3}A_{2\alpha}$		+1Li
456.2416	0.46	1	456.2415	0.11	$^{2,4}A_{2\alpha}$		+1Li
458.2458	1.11	1	458.2458	-0.04	$Y_{1\alpha}$	-2H	+1Li
460.2615	0.30	1	460.2614	0.11	$Y_{1\alpha}$		+1Li
466.2696	1.15	1	466.2696	-0.09	$Y_{1\alpha}$	-H	+2Li
471.2404	0.14	2	942.4828	-2.20	$^{3,5}X_{1\alpha}$	-2H	+2Li
485.2573	0.37	2	970.5141	0.50	$^{0,4}X_{1\alpha}$	-2H	+2Li
485.2573	0.37	2	970.5141	0.50	$^{0,4}X_{0}$	-2H	+2Li
486.2647	1.42	2	972.5248	4.74	$^{1,5}A_{3}$	2H	0

486.2647	1.42	2	972.5297	-0.34	$^{0,4}X_{1\alpha}$		+2Li
486.2647	1.42	2	972.5297	-0.34	$^{0,4}X_0$		+2Li
488.2564	1.52	1	488.2563	0.10	$^{1,5}X_{1\alpha}$		+1Li
491.7638	0.10	2	983.5244	3.31	$^{1,3}X_{2\alpha}$	2H	+1Li
493.2547	0.09	2	986.5090	0.37	$^{1,3}X_{2\alpha}$	-2H	+2Li
494.2620	0.16	2	988.5247	-0.70	$^{1,3}X_{2\alpha}$		+2Li
500.2619	0.21	2	1000.5197	4.06	B_3	2H	0
500.2619	0.21	2	1000.5247	-0.85	$^{0,4}X_{1\beta}$	-2H	+2Li
501.2695	0.37	2	1002.5403	-1.30	$^{0,4}X_{1\beta}$		+2Li
501.7744	0.15	2	1003.5482	0.69	$^{0,4}X_{1\beta}$	H	+2Li
512.2679	0.06	1	512.2678	0.20	$^{2,5}A_{2\alpha}$	-2H	+1Li
516.2875	0.22	1	516.2877	-0.38	$^{0,2}X_{1\alpha}$		+1Li
538.2909	0.03	1	538.2908	0.21	$^{2,5}X_{1\alpha}$	-H	+2Li
556.2940	0.50	1	556.2940	0.02	$^{1,5}A_{2\alpha}$	-2H	+1Li
558.3101	0.07	1	558.3096	0.85	$^{1,5}A_{2\alpha}$		+1Li
586.3045	0.11	1	586.3046	-0.12	$B_{2\alpha}$		+1Li
588.3089	0.10	1	588.3088	0.13	$^{1,3}X_{1\alpha}$	-2H	+1Li
588.3089	0.10	1	588.3088	0.13	$^{2,4}X_{1\alpha}$	-2H	+1Li
590.3246	0.10	1	590.3245	0.19	$^{1,3}X_{1\alpha}$		+1Li
590.3246	0.10	1	590.3245	0.19	$^{2,4}X_{1\alpha}$		+1Li
596.3323	0.12	1	596.3326	-0.63	$^{1,3}X_{1\alpha}$	-H	+2Li
596.3323	0.12	1	596.3326	-0.63	$^{2,4}X_{1\alpha}$	-H	+2Li
602.2994	1.03	1	602.2995	-0.18	$C_{2\alpha}$	-2H	+1Li
610.3228	0.14	1	610.3233	-0.82	$C_{2\alpha}$	-H	+2Li
638.3433	2.42	1	638.3432	0.21	$Z_{2\alpha}$	$-CH_3$	+2Li
662.3463	1.32	1	662.3456	1.13	$Y_{2\alpha}$	-2H	+1Li
664.3613	4.43	1	664.3612	0.17	$Y_{2\alpha}$		+1Li
670.3694	5.45	1	670.3694	-0.02	$Y_{2\alpha}$	-H	+2Li
674.3569	0.12	1	674.3570	-0.20	$^{3,5}A_3$		+1Li
734.3669	0.20	1	734.3667	0.27	$^{1,3}X_0$	-2H	+1Li
748.3824	0.48	1	748.3823	0.07	$^{0,2}X_{2\alpha}$		+1Li
750.3618	0.24	1	750.3616	0.23	$^{1,5}X_{2\alpha}$		+1Li
833.4354	0.24	1	833.4351	0.35	$Z_{1\beta}$		+1Li
857.4541	0.34	1	857.4539	0.27	$Y_{1\beta}$	-H	+2Li
924.4881	0.07	1	924.4836	4.82	$^{1,4}A_3$	-2H	+2Li
981.5074	0.05	1	981.5087	-1.32	$^{1,3}X_{2\alpha}$		+1Li
1013.5328	0.15	1	1013.5349	-2.09	$^{1,3}X_{2\alpha}$	OCH_4	+1Li
1045.5593	0.20	1	1045.5587	0.60	$^{0,4}X_{1\beta}$	OC_2H_3	+2Li

Table S5. List of ECD fragment ions of the doubly lithiated, permethylated, and ^{18}O-Labeled Sialyl Lewis A at *m/z* 523.2830.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
376.1969	0.02	1	376.1966	0.78	$B_{1\alpha}$	H	0
406.2236	0.87	1	406.2235	0.20	$C_{1\alpha}$	-H	+2Li
419.2553	0.68	1	419.2563	-2.45	$Z_{1\alpha}$	$-OCH_2$	+2Li
460.2616	0.09	1	460.2614	0.31	$Y_{1\alpha}$		+1Li
466.2695	1.06	1	466.2696	-0.29	$Y_{1\alpha}$	-H	+2Li
520.2916	0.31	1	520.2916	0.04	$^{2,5}A_{2\alpha}$	-H	+2Li
536.2865	0.05	1	536.2865	-0.02	$^{0,2}A_{2\alpha}$	-H	+2Li
566.3221	0.91	1	566.3221	-0.01	$^{2,4}X_{1\alpha}$	$-OCH_3$	+2Li
566.3221	0.91	1	566.3221	-0.01	$^{1,3}X_{1\alpha}$	$-OCH_3$	+2Li
602.2997	0.15	1	602.2995	0.33	$C_{2\alpha}$	-2H	+1Li
610.3234	0.19	1	610.3233	0.18	$C_{2\alpha}$	-H	+2Li
654.3739	0.05	1	654.3745	-0.89	$Z_{2\alpha}$	H	+2Li
664.3607	0.43	1	664.3612	-0.75	$Y_{2\alpha}$		+1Li
670.3695	5.41	1	670.3694	0.17	$Y_{2\alpha}$	-H	+2Li
748.3828	0.03	1	748.3823	0.64	$^{0,2}X_{2\alpha}$		+1Li
821.4325	0.14	1	821.4351	-3.20	$Y_{1\beta}$	$-OCH_2$	+1Li
843.4747	0.28	1	843.4746	0.07	$Z_{1\beta}$	3H	+2Li
851.4429	0.03	1	851.4457	-3.31	$Y_{1\beta}$		+1Li
857.4537	0.03	1	857.4539	-0.23	$Y_{1\beta}$	-H	+2Li
912.4854	0.04	1	912.4872	-1.98	$^{2,4}X_{2\alpha}$	2H	+1Li
951.4956	0.07	1	951.4981	-2.64	$^{0,3}X_{1\beta}$		+1Li
951.4956	0.07	1	951.4981	-2.64	$^{1,3}X_{1\beta}$		+1Li
951.4956	0.07	1	951.4981	-2.64	$^{2,4}X_{1\beta}$		+1Li
969.5031	0.07	1	969.5013	1.84	$^{1,5}A_3$	-H	0
983.5220	0.11	1	983.5244	-2.40	$^{1,3}X_{2\alpha}$	2H	+1Li
999.5167	0.11	1	999.5119	4.81	B_3	H	0

Table S6. List of EED fragment ions of the doubly lithiated, permethylated, and ^{18}O-Labeled Sialyl Lewis A at *m/z* 523.2830.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
211.1150	0.32	1	211.1152	-1.09	$C_{1\beta}$	-2H	+1Li
213.1306	0.19	1	213.1309	-1.34	$C_{1\beta}$		+1Li
219.1388	0.36	1	219.1391	-1.24	$C_{1\beta}$	-H	+2Li
236.1467	0.16	1	236.1469	-0.72	$^{3,5}A_{1\alpha}$	-2H	+1Li
238.1623	0.24	1	238.1625	-0.95	$^{3,5}A_{1\alpha}$		+1Li
252.1415	0.05	1	252.1418	-1.10	$^{0,3}A_{1\alpha}$	-2H	+1Li
280.1728	0.08	1	280.1731	-1.04	$^{2,5}A_{1\alpha}$	-2H	+1Li
283.1727	0.15	1	283.1727	-0.15	$^{3,5}A_{3}$		+1Li
294.1885	0.07	1	294.1888	-0.78	$^{1,5}A_{1\alpha}$	-2H	+1Li
296.2042	0.03	1	296.2044	-0.66	$^{1,5}A_{1\alpha}$		+1Li
297.1769	0.05	1	297.1758	3.70	$^{0,2}A_{1\alpha}$	-H	+1Li
340.1941	4.28	1	340.1942	-0.36	$^{1,3}X_{2\alpha}/B_{2\alpha}$	CH_4	+1Li
376.1966	5.20	1	376.1966	-0.03	$B_{1\alpha}$	H	0
377.6989	0.18	2	755.3983	-0.68	$^{0,2}X_{2\alpha}$		+2Li
382.2048	2.67	1	382.2048	0.05	$B_{1\alpha}$		+1Li
383.2126	0.53	1	383.2126	-0.06	$B_{1\alpha}$	H	+1Li
384.2204	0.11	1	384.2204	-0.10	$B_{1\alpha}$	2H	+1Li
388.2129	0.05	1	388.2130	-0.19	$B_{1\alpha}$	-H	+2Li
390.2286	0.07	1	390.2286	-0.01	$B_{1\alpha}$	H	+2Li
398.1997	0.09	1	398.1997	0.03	$C_{1\alpha}$	-2H	+1Li
400.2155	0.14	1	400.2153	0.43	$C_{1\alpha}$		+1Li
406.2235	0.81	1	406.2235	-0.03	$C_{1\alpha}$	-H	+2Li
420.2256	0.10	2	840.4511	0.04	$Z_{1\beta}$		+2Li
428.2231	0.07	2	856.4460	0.21	$Y_{1\beta}$	-2H	+2Li
436.2428	0.44	1	436.2427	0.18	$Z_{1\alpha}$	H	0
442.2508	8.87	1	442.2509	-0.23	$Z_{1\alpha}$		+1Li
443.2279	0.42	2	886.4566	-0.92	$^{1,5}X_{1\beta}$		+2Li
456.2417	0.16	2	912.4872	-4.19	$^{2,4}X_{2\alpha}$	2H	+1Li
457.2443	0.14	2	914.4879	0.77	$^{0,2}X_{1\beta}$		+2Li
457.2443	0.14	2	914.4879	0.77	$^{1,4}X_{1\beta}$		+2Li
458.2458	0.41	1	458.2458	-0.04	$Y_{1\alpha}$	-2H	+1Li
460.2615	0.27	1	460.2614	0.11	$Y_{1\alpha}$		+1Li

464.2655	0.21	1	464.2654	0.25	$^{1,3}A_{2\alpha}$	H	+2Li
464.2655	0.21	1	464.2654	0.25	$^{2,4}A_{2\alpha}$	H	+2Li
466.2696	1.42	1	466.2696	-0.09	$Y_{1\alpha}$	-H	+2Li
485.2573	0.35	2	970.5141	0.50	$^{0,4}X_{1\alpha}$	-2H	+2Li
485.2573	0.35	2	970.5141	0.50	$^{0,4}X_{0}$	-2H	+2Li
486.2647	2.17	2	972.5248	4.74	$^{1,5}A_{3}$	2H	0
486.2647	2.17	2	972.5297	-0.34	$^{0,4}X_{1\alpha}$		+2Li
486.2647	2.17	2	972.5297	-0.34	$^{0,4}X_{0}$		+2Li
488.2563	1.22	1	488.2563	-0.15	$^{1,5}X_{1\alpha}$		+1Li
491.7638	0.11	2	983.5244	3.31	$^{1,3}X_{2\alpha}$	2H	+1Li
493.2549	0.08	2	986.5090	0.81	$^{1,3}X_{2\alpha}$	-2H	+2Li
494.2620	0.12	2	988.5247	-0.70	$^{1,3}X_{2\alpha}$		+2Li
500.2626	0.26	2	1000.5247	0.55	$^{0,4}X_{1\beta}$	-2H	+2Li
501.2711	0.22	2	1002.5403	1.86	$^{0,4}X_{1\beta}$		+2Li
501.7742	0.04	2	1003.5482	0.27	$^{0,4}X_{1\beta}$	H	+2Li
512.2680	0.06	1	512.2678	0.44	$^{2,5}A_{2\alpha}$	-2H	+1Li
514.2833	0.08	1	514.2834	-0.20	$^{2,5}A_{2\alpha}$		+1Li
516.2876	0.10	1	516.2877	-0.14	$^{0,2}X_{1\alpha}$		+1Li
520.2916	0.34	1	520.2916	0.04	$^{2,5}A_{2\alpha}$	-H	+2Li
528.2629	0.03	1	528.2627	0.37	$^{0,2}A_{2\alpha}$	-2H	+1Li
530.2785	0.08	1	530.2783	0.32	$^{0,2}A_{2\alpha}$		+1Li
532.2827	0.07	1	532.2826	0.21	$^{2,5}X_{1\alpha}$		+1Li
546.2982	0.44	1	546.2982	-0.02	$^{1,4}X_{1\alpha}$		+1Li
556.2941	0.36	1	556.2940	0.24	$^{1,5}A_{2\alpha}$	-2H	+1Li
558.3097	0.06	1	558.3096	0.09	$^{1,5}A_{2\alpha}$		+1Li
586.3046	0.09	1	586.3046	0.08	$B_{2\alpha}$		+1Li
588.3092	0.06	1	588.3088	0.65	$^{1,3}X_{1\alpha}$	-2H	+1Li
588.3092	0.06	1	588.3088	0.65	$^{2,4}X_{1\alpha}$	-2H	+1Li
590.3241	0.07	1	590.3245	-0.64	$^{1,3}X_{1\alpha}$		+1Li
590.3241	0.07	1	590.3245	-0.64	$^{2,4}X_{1\alpha}$		+1Li
596.3326	0.06	1	596.3326	-0.12	$^{1,3}X_{1\alpha}$	-H	+2Li
596.3326	0.06	1	596.3326	-0.12	$^{2,4}X_{1\alpha}$	-H	+2Li
602.2995	1.26	1	602.2995	0.02	$C_{2\alpha}$	-2H	+1Li
604.3152	0.22	1	604.3151	0.08	$C_{2\alpha}$		+1Li
610.3234	0.15	1	610.3233	0.18	$C_{2\alpha}$	-H	+2Li
616.3401	1.01	1	616.3401	-0.01	$Z_{2\alpha}$	$-OCH_2$	+1Li
646.3506	0.35	1	646.3506	-0.11	$Z_{2\alpha}$		+1Li
662.3460	0.65	1	662.3456	0.67	$Y_{2\alpha}$	-2H	+1Li
664.3612	3.00	1	664.3612	-0.02	$Y_{2\alpha}$		+1Li
670.3695	1.35	1	670.3694	0.17	$Y_{2\alpha}$	-H	+2Li

748.3824	0.62	1	748.3823	0.07	$^{0,2}X_{2\alpha}$		+1Li
750.3617	0.14	1	750.3616	0.07	$^{1,5}X_{2\alpha}$		+1Li
761.3775	0.05	1	761.3776	-0.14	$^{3,5}X_{0}$	-2H	+1Li
833.4349	0.17	1	833.4351	-0.31	$Z_{1\beta}$		+1Li
857.4542	0.34	1	857.4539	0.41	$Y_{1\beta}$	-H	+2Li
879.4416	0.03	1	879.4406	1.10	$^{1,5}X_{1\beta}$		+1Li
965.5149	0.07	1	965.5137	1.19	$^{0,4}X_{1\alpha}$		+1Li
965.5149	0.07	1	965.5137	1.19	$^{0,4}X_{0}$		+1Li
981.5071	0.03	1	981.5087	-1.63	$^{1,3}X_{2\alpha}$		+1Li

Table S7. List of ECD fragment ions of the doubly lithiated, permethylated, ^{18}O-labeled LNT at *m/z* 459.7513.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
249.1502	0.32	1	249.1496	2.34	C_1	-H	+2Li
251.1544	0.27	1	251.1539	2.14	Y_1	-H	+2Li
279.1492	1.37	1	279.1488	1.49	$^{1,5}X_1$	-H	+2Li
305.1762	0.03	1	305.1758	1.26	$^{2,4}A_2$	-H	+2Li
307.1804	0.14	1	307.1801	0.96	$^{0,2}X_1$	-H	+2Li
337.1909	0.03	1	337.1906	0.69	$^{1,4}X_1$	-H	+2Li
339.2065	0.04	1	339.2063	0.61	$^{1,4}X_1$	H	+2Li
346.2026	0.03	1	346.2024	0.67	$^{1,3}A_2$	-H	+2Li
363.2179	0.29	1	363.2177	0.56	$^{2,5}A_2$	-H	+2Li
381.2171	0.15	1	381.2169	0.61	$^{1,3}X_1$	-H	+2Li
381.2171	0.15	1	381.2169	0.61	$^{2,4}X_1$	-H	+2Li
431.2350	0.70	1	431.2349	0.18	Z_2		+1Li
439.2587	0.03	1	439.2587	-0.08	Z_2	H	+2Li
447.2308	0.03	1	447.2298	2.21	Y_2	-2H	+1Li
448.2375	0.79	1	448.2376	-0.34	Y_2	-H	+1Li
449.2457	0.13	1	449.2455	0.52	Y_2		+1Li
450.2862	0.40	1	450.2861	0.19	$^{1,5}A_2$	H	+2Li
450.7329	0.04	2	901.4677	-2.03	C_4	-2H	+2Li
455.2536	3.76	1	455.2536	-0.09	Y_2	-H	+2Li
464.2491	0.15	1	464.2490	0.17	B_2	H	0
470.2572	0.03	1	470.2572	-0.03	B_2		+1Li
478.2809	2.67	1	478.2810	-0.27	B_2	H	+2Li
494.2758	0.34	1	494.2759	-0.33	C_2	-H	+2Li
581.3213	0.03	1	581.3242	-4.89	$^{1,3}X_2$	2H	+1Li
594.3279	0.04	1	594.3284	-0.84	$^{1,4}A_3$	-H	+2Li
652.3698	0.10	1	652.3702	-0.67	$^{1,5}A_3$	-H	+2Li
678.3764	0.02	1	678.3769	-0.68	Z_3	2H	+1Li
682.3800	0.11	1	682.3809	-1.22	B_3	H	+2Li
684.3847	2.95	1	684.3851	-0.50	Z_3	H	+2Li
698.3754	0.27	1	698.3757	-0.45	C_3	-H	+2Li
700.3797	0.24	1	700.3799	-0.36	Y_3	-H	+2Li
779.4130	0.35	1	779.4121	1.14	$^{0,3}A_4$	H	+1Li

782.4212	0.02	1	782.4243	-3.87	$^{1,4}X_3$	2H	+1Li
785.4218	0.04	1	785.4203	1.91	$^{0,3}A_4$		+2Li
826.4483	0.05	1	826.4504	-2.56	$^{1,3}X_3$	2H	+1Li
826.4483	0.05	1	826.4504	-2.56	$^{1,3}X_0$	2H	+1Li
826.4483	0.05	1	826.4504	-2.56	$^{2,4}X_3$	2H	+1Li
896.4670	0.97	1	896.4673	-0.35	C_4		+1Li

Table S8. List of EED fragment ions of the doubly lithiated, permethylated, ^{18}O-labeled LNT at *m/z* 459.7513.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
195.1204	0.30	1	195.1203	0.46	$^{1,5}A_1$	-2H	+1Li
197.1360	0.11	1	197.1360	0.17	$^{1,5}A_1$		+1Li
225.1309	0.31	1	225.1309	0.08	B_1		+1Li
227.1352	0.71	1	227.1351	0.28	Z_1		+1Li
241.1258	2.55	1	241.1258	-0.01	C_1	-2H	+1Li
243.1415	1.57	1	243.1414	0.20	C_1		+1Li
245.1458	0.51	1	245.1457	0.45	Y_1		+1Li
249.1497	2.66	1	249.1496	0.32	C_1	-H	+2Li
251.1539	3.92	1	251.1539	0.14	Y_1	-H	+2Li
273.1405	2.26	1	273.1406	-0.38	$^{1,5}X_1$		+1Li
299.1676	0.18	1	299.1676	-0.14	$^{2,4}A_2$		+1Li
301.1718	0.36	1	301.1719	-0.34	$^{0,2}X_1$		+1Li
307.1801	0.21	1	307.1801	0.06	$^{0,2}X_1$	-H	+2Li
325.6814	0.14	2	651.3624	0.56	$^{1,5}A_3$	-2H	+2Li
338.6841	0.40	2	677.3690	-1.21	Z_3	H	+1Li
340.1942	0.14	1	340.1942	0.05	$^{1,3}A_2$		+1Li
349.6914	0.14	2	699.3835	-1.08	C_3		+2Li
355.1939	0.12	1	355.1939	0.12	$^{2,5}A_2$	-2H	+1Li
359.2252	0.11	1	359.2252	0.07	$^{2,5}A_2$	2H	+1Li
364.6911	0.73	2	729.3827	-0.70	$^{1,5}X_3$		+2Li
377.7044	0.13	2	755.4097	-1.24	$^{2,4}A_4$		+2Li
378.7067	0.10	2	757.4140	-0.84	$^{0,2}X_3$		+2Li
382.2046	0.11	1	382.2048	-0.44	$^{1,4}A_2$	-2H	+1Li
384.7123	1.04	2	769.4254	-1.06	$^{3,5}A_4$		+2Li
391.2125	0.13	2	782.4243	0.97	$^{1,4}X_3$	2H	+1Li
421.7254	1.03	2	843.4508	0.00	$^{0,4}X_3$	-2H	+2Li
421.7254	1.03	2	843.4508	0.00	$^{0,4}X_2$	-2H	+2Li
421.7254	1.03	2	843.4508	0.00	$^{0,4}X_1$	-2H	+2Li
421.7254	1.03	2	843.4508	0.00	$^{0,4}X_0$	-2H	+2Li
422.7327	1.21	2	845.4664	-1.26	$^{0,4}X_3$		+2Li
422.7327	1.21	2	845.4664	-1.26	$^{0,4}X_2$		+2Li

422.7327	1.21	2	845.4664	-1.26	$^{0,4}X_1$		+2Li
422.7327	1.21	2	845.4664	-1.26	$^{0,4}X_0$		+2Li
428.7386	1.61	2	857.4778	-0.81	$^{1,5}A_4$		+2Li
431.2350	2.13	1	431.2349	0.18	Z_2		+1Li
440.2468	0.17	1	440.2466	0.38	$^{1,5}A_2$	-2H	+1Li
442.2623	0.55	1	442.2623	0.04	$^{1,5}A_2$		+1Li
447.2298	1.15	1	447.2298	-0.04	Y_2	-2H	+1Li
449.2454	6.63	1	449.2455	-0.16	Y_2		+1Li
455.2536	7.65	1	455.2536	-0.09	Y_2	-H	+2Li
464.2490	1.33	1	464.2490	-0.09	B_2	H	0
470.2571	6.11	1	470.2572	-0.22	B_2		+1Li
477.2403	3.53	1	477.2404	-0.15	$^{1,5}X_2$		+1Li
486.2520	3.04	1	486.2521	-0.22	C_2	-2H	+1Li
488.2678	0.18	1	488.2678	0.04	C_2		+1Li
544.2939	0.35	1	544.2939	-0.13	$^{1,3}A_3$		+1Li
544.2939	0.35	1	544.2939	-0.13	$^{2,4}A_3$		+1Li
573.2985	0.14	1	573.3003	-3.11	$^{1,3}X_2$	H	0
588.3200	0.12	1	588.3202	-0.33	$^{1,4}A_3$		+1Li
594.3282	0.14	1	594.3284	-0.33	$^{1,4}A_3$	-H	+2Li
600.3206	0.11	1	600.3202	0.73	$^{2,5}A_3$	-2H	+1Li
602.3340	0.18	1	602.3358	-3.06	$^{2,5}A_3$		+1Li
620.3352	0.12	1	620.3350	0.28	$^{2,4}X_2$		+1Li
644.3466	0.98	1	644.3464	0.30	$^{1,5}A_3$	-2H	+1Li
670.3533	0.25	1	670.3530	0.35	Z_3	H	0
674.3571	0.27	1	674.3570	0.16	B_3		+1Li
676.3614	2.52	1	676.3612	0.25	Z_3		+1Li
690.3519	1.21	1	690.3519	0.02	C_3	-2H	+1Li
692.3568	0.17	1	692.3561	0.99	Y_3	-2H	+1Li
694.3725	0.14	1	694.3718	1.04	Y_3		+1Li
698.3759	0.19	1	698.3757	0.25	C_3	-H	+2Li
722.3673	0.93	1	722.3667	0.83	$^{1,5}X_3$		+1Li
896.4683	0.16	1	896.4673	1.14	C_4		+1Li

Table S9. List of EED fragment ions of the singly lithiated, permethylated, ^{18}O-labeled LNT at *m/z* 912.4872.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
225.1306	0.04	1	225.1309	-1.27	B_1		+1Li
227.1349	0.07	1	227.1351	-0.99	Z_1		+1Li
243.1413	0.27	1	243.1414	-0.61	C_1		+1Li
245.1455	0.09	1	245.1457	-0.80	Y_1		+1Li
273.1406	0.24	1	273.1406	-0.04	$^{1,5}X_1$		+1Li
299.1677	0.04	1	299.1676	0.16	$^{2,4}A_2$		+1Li
301.1720	0.03	1	301.1719	0.26	$^{0,2}X_1$		+1Li
340.1944	0.08	1	340.1942	0.59	$^{1,3}A_2$		+1Li
355.1942	0.02	1	355.1939	0.98	$^{2,5}A_2$	-2H	+1Li
382.2051	0.04	1	382.2048	0.91	$^{1,4}A_2$	-2H	+1Li
431.2354	1.37	1	431.2349	1.18	Z_2		+1Li
440.2472	0.13	1	440.2466	1.28	$^{1,5}A_2$	-2H	+1Li
442.2628	0.37	1	442.2623	1.15	$^{1,5}A_2$		+1Li
449.2460	6.54	1	449.2455	1.20	Y_2		+1Li
464.2496	0.09	1	464.2490	1.22	B_2	H	0
470.2576	2.91	1	470.2572	0.82	B_2		+1Li
477.2409	1.47	1	477.2404	1.13	$^{1,5}X_2$		+1Li
486.2526	1.49	1	486.2521	0.97	C_2	-2H	+1Li
487.2607	0.07	1	487.2599	1.57	C_2	-H	+1Li
488.2683	0.07	1	488.2678	1.10	C_2		+1Li
544.2946	0.17	1	544.2939	1.21	$^{1,3}A_3$		+1Li
544.2946	0.17	1	544.2939	1.21	$^{2,4}A_3$		+1Li
546.2988	0.03	1	546.2982	1.10	$^{0,2}X_2$		+1Li
561.2860	0.02	1	561.2853	1.20	$^{2,5}X_2$	-H	+1Li
573.2979	0.01	1	573.2968	2.07	$^{1,4}A_3$	$-CH_3$	+1Li
574.2939	0.05	1	574.2932	1.25	$^{2,4}X_2$	$-OC_2H_6$	+1Li
600.3209	0.02	1	600.3202	1.24	$^{2,5}A_3$	-2H	+1Li
612.3207	0.01	1	612.3226	-3.11	$^{0,2}A_3$	H	0
614.3252	0.02	1	614.3268	-2.70	$^{2,4}X_2$	H	0
620.3357	0.11	1	620.3350	1.06	$^{2,4}X_2$		+1Li
644.3471	0.57	1	644.3464	1.06	$^{1,5}A_3$	-2H	+1Li
670.3537	0.03	1	670.3530	0.98	Z_3	H	0

675.3655	0.03	1	675.3648	0.96	B_3	H	+1Li
676.3618	1.41	1	676.3612	0.88	Z_3		+1Li
677.3718	0.08	1	677.3690	4.11	Z_3	H	+1Li
690.3524	0.88	1	690.3519	0.73	C_3	-2H	+1Li
692.3576	0.30	1	692.3561	2.14	Y_3	-2H	+1Li
694.3726	0.03	1	694.3718	1.21	Y_3		+1Li
722.3675	1.06	1	722.3667	1.08	$^{1,5}X_3$		+1Li
748.3946	0.02	1	748.3937	1.13	$^{2,4}A_4$		+1Li
750.3986	0.03	1	750.3980	0.80	$^{0,2}X_3$		+1Li
761.4040	0.01	1	761.4016	3.13	$^{3,5}A_4$	-H	+1Li
762.4101	0.40	1	762.4094	0.86	$^{3,5}A_4$		+1Li
766.3937	0.03	1	766.3929	1.02	$^{2,5}X_3$		+1Li
778.3945	0.04	1	778.3929	1.98	$^{1,4}X_3$	-2H	+1Li
780.4093	0.02	1	780.4086	0.92	$^{1,4}X_3$		+1Li
794.4252	0.02	1	794.4242	1.21	$^{0,3}X_3$		+1Li
794.4252	0.02	1	794.4242	1.21	$^{0,3}X_2$		+1Li
794.4252	0.02	1	794.4242	1.21	$^{0,3}X_1$		+1Li
804.4206	0.02	1	804.4200	0.78	$^{2,5}A_4$	-2H	+1Li
808.4042	0.03	1	808.4035	0.85	$^{3,5}X_3$	-2H	+1Li
808.4042	0.03	1	808.4035	0.85	$^{3,5}X_2$	-2H	+1Li
808.4042	0.03	1	808.4035	0.85	$^{3,5}X_1$	-2H	+1Li
822.4206	0.02	1	822.4191	1.80	$^{1,3}X_3$	-2H	+1Li
822.4206	0.02	1	822.4191	1.80	$^{1,3}X_0$	-2H	+1Li
822.4206	0.02	1	822.4191	1.80	$^{2,4}X_3$	-2H	+1Li
836.4363	0.57	1	836.4348	1.77	$^{0,4}X_3$	-2H	+1Li
836.4363	0.57	1	836.4348	1.77	$^{0,4}X_2$	-2H	+1Li
836.4363	0.57	1	836.4348	1.77	$^{0,4}X_1$	-2H	+1Li
836.4363	0.57	1	836.4348	1.77	$^{0,4}X_0$	-2H	+1Li
838.4509	0.32	1	838.4504	0.57	$^{0,4}X_3$		+1Li
838.4509	0.32	1	838.4504	0.57	$^{0,4}X_2$		+1Li
838.4509	0.32	1	838.4504	0.57	$^{0,4}X_1$		+1Li
838.4509	0.32	1	838.4504	0.57	$^{0,4}X_0$		+1Li
848.4476	0.20	1	848.4462	1.60	$^{1,5}A_4$	-2H	+1Li
850.4623	0.59	1	850.4619	0.49	$^{1,5}A_4$		+1Li

Table S10. List of EED fragment ions of the singly cesiated, permethylated, ^{18}O-labeled LNT at *m/z* 1038.3767.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
205.9340	0.01	1	205.9339	0.70	$^{0,4}A_1$	-H	+1Cs
205.9340	0.01	1	205.9339	0.70	$^{0,4}A_2$	-H	+1Cs
205.9340	0.01	1	205.9339	0.70	$^{0,4}A_3$	-H	+1Cs
205.9340	0.01	1	205.9339	0.70	$^{0,4}A_4$	-H	+1Cs
278.9994	0.02	1	278.9992	0.66	$^{2,5}A_1$		+1Cs
321.0101	0.02	1	321.0098	1.05	$^{1,5}A_1$	-2H	+1Cs
322.0182	0.01	1	322.0176	1.85	$^{1,5}A_1$	-H	+1Cs
323.0257	0.07	1	323.0254	0.85	$^{1,5}A_1$		+1Cs
351.0205	0.02	1	351.0203	0.48	B_1		+1Cs
352.0283	0.01	1	352.0282	0.35	B_1	H	+1Cs
353.0249	0.34	1	353.0246	0.91	Z_1		+1Cs
367.0163	0.13	1	367.0153	2.87	C_1	-2H	+1Cs
368.0234	0.04	1	368.0231	0.91	C_1	-H	+1Cs
369.0312	0.13	1	369.0309	0.79	C_1		+1Cs
399.0304	0.14	1	399.0301	0.84	$^{1,5}X_1$		+1Cs
464.2494	0.08	1	464.2490	0.76	B_2	H	0
466.0839	0.07	1	466.0836	0.52	$^{1,3}A_2$		+1Cs
481.0836	0.02	1	481.0833	0.57	$^{2,5}A_2$	-2H	+1Cs
485.1148	0.01	1	485.1146	0.38	$^{2,5}A_2$	2H	+1Cs
508.0945	0.02	1	508.0942	0.60	$^{1,4}A_2$	-2H	+1Cs
557.1250	1.52	1	557.1244	1.15	Z_2		+1Cs
566.1376	0.03	1	566.1361	2.64	$^{1,5}A_2$	-2H	+1Cs
568.1519	0.05	1	568.1517	0.32	$^{1,5}A_2$		+1Cs
573.1199	0.48	1	573.1193	1.06	Y_2	-2H	+1Cs
575.1352	0.24	1	575.1349	0.48	Y_2		+1Cs
596.1469	0.17	1	596.1467	0.41	B_2		+1Cs
597.1548	0.10	1	597.1545	0.49	B_2	H	+1Cs
603.1299	1.62	1	603.1298	0.10	$^{1,5}X_2$		+1Cs
612.1417	2.21	1	612.1416	0.25	C_2	-2H	+1Cs
613.1521	0.06	1	613.1494	4.40	C_2	-H	+1Cs
670.1833	0.17	1	670.1834	-0.18	$^{1,3}A_3$		+1Cs
670.1833	0.17	1	670.1834	-0.18	$^{2,4}A_3$		+1Cs

670.3529	0.05	1	670.3530	-0.20	Z_3	H	0
686.1682	0.02	1	686.1670	1.82	$^{2,5}X_2$	-2H	+1Cs
687.1745	0.03	1	687.1748	-0.42	$^{2,5}X_2$	-H	+1Cs
726.2096	0.02	1	726.2096	-0.04	$^{2,5}A_3$	-2H	+1Cs
729.2305	0.07	1	729.2331	-3.54	$^{2,5}A_3$	H	+1Cs
746.2237	0.22	1	746.2245	-1.06	$^{2,4}X_2$		+1Cs
770.2353	0.46	1	770.2358	-0.75	$^{1,5}A_3$	-2H	+1Cs
800.2436	0.02	1	800.2465	-3.58	B_3		+1Cs
802.2506	0.86	1	802.2507	-0.08	Z_3		+1Cs
816.2407	1.92	1	816.2413	-0.79	C_3	-2H	+1Cs
818.2461	0.52	1	818.2456	0.63	Y_3	-2H	+1Cs
848.2531	0.90	1	848.2562	-3.60	$^{1,5}X_3$		+1Cs
874.2821	0.04	1	874.2832	-1.26	$^{2,4}A_4$		+1Cs
876.2865	0.04	1	876.2875	-1.11	$^{0,2}X_3$		+1Cs
888.2980	0.54	1	888.2989	-1.03	$^{3,5}A_4$		+1Cs
904.2828	0.02	1	904.2823	0.44	$^{1,4}X_3$	-2H	+1Cs
906.2969	0.03	1	906.2980	-1.28	$^{1,4}X_3$		+1Cs
920.3127	0.03	1	920.3137	-1.06	$^{0,3}X_3$		+1Cs
920.3127	0.03	1	920.3137	-1.06	$^{0,3}X_2$		+1Cs
920.3127	0.03	1	920.3137	-1.06	$^{0,3}X_1$		+1Cs
930.3084	0.02	1	930.3094	-1.08	$^{2,5}A_4$	-2H	+1Cs
962.3242	0.55	1	962.3242	-0.03	$^{0,4}X_3$	-2H	+1Cs
962.3242	0.55	1	962.3242	-0.03	$^{0,4}X_2$	-2H	+1Cs
962.3242	0.55	1	962.3242	-0.03	$^{0,4}X_1$	-2H	+1Cs
962.3242	0.55	1	962.3242	-0.03	$^{0,4}X_0$	-2H	+1Cs
964.3387	0.31	1	964.3399	-1.27	$^{0,4}X_3$		+1Cs
964.3387	0.31	1	964.3399	-1.27	$^{0,4}X_2$		+1Cs
964.3387	0.31	1	964.3399	-1.27	$^{0,4}X_1$		+1Cs
964.3387	0.31	1	964.3399	-1.27	$^{0,4}X_0$		+1Cs
974.3338	0.25	1	974.3357	-1.91	$^{1,5}A_4$	-2H	+1Cs
976.3515	0.42	1	976.3513	0.19	$^{1,5}A_4$		+1Cs

Table S11. List of ECD fragment ions of the doubly lithiated, permethylated, ^{18}O-labeled LNnT at *m/z* 459.7513.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
249.1496	0.18	1	249.1496	-0.11	C_1	-H	+2Li
251.1538	0.34	1	251.1539	-0.29	Y_1	-H	+2Li
279.1487	1.05	1	279.1488	-0.26	$^{1,5}X_1$	-H	+2Li
307.1801	0.10	1	307.1801	0.06	$^{0,2}X_1$	-H	+2Li
317.1760	0.23	1	317.1758	0.52	$^{3,5}A_2$	-3H	+2Li
321.1600	0.05	1	321.1594	2.04	$^{2,5}X_1$	-3H	+2Li
351.2003	0.16	1	351.2013	-2.99	$^{2,5}A_2$	H	0
361.2021	0.12	1	361.2021	0.12	$^{2,5}A_2$	-3H	+2Li
363.2177	0.15	1	363.2177	0.05	$^{2,5}A_2$	-H	+2Li
381.2169	0.13	1	381.2169	0.05	$^{1,3}X_1$	-H	+2Li
381.2169	0.13	1	381.2169	0.05	$^{2,4}X_1$	-H	+2Li
388.2130	0.76	1	388.2130	0.19	$^{1,4}A_2$	-3H	+2Li
431.2349	1.60	1	431.2349	-0.03	Z_2		+1Li
447.2308	0.07	1	447.2298	2.21	Y_2	-2H	+1Li
448.2376	0.71	1	448.2376	-0.07	Y_2	-H	+1Li
450.2298	0.04	2	900.4598	-0.26	C_4	-3H	+2Li
450.2862	0.25	1	450.2861	0.19	$^{1,5}A_2$	H	+2Li
451.2364	0.03	2	902.4755	-2.99	C_4	-H	+2Li
453.2381	2.00	1	453.2380	0.23	Y_2	-3H	+2Li
455.2536	6.72	1	455.2536	-0.09	Y_2	-H	+2Li
464.2491	0.28	1	464.2490	0.17	B_2	H	0
470.2572	0.09	1	470.2572	-0.03	B_2		+1Li
478.2811	4.99	1	478.2810	0.12	B_2	H	+2Li
494.2759	0.11	1	494.2759	-0.08	C_2	-H	+2Li
545.3035	0.06	1	545.3018	3.20	$^{1,3}A_3$	H	+1Li
545.3035	0.06	1	545.3018	3.20	$^{2,4}A_3$	H	+1Li
554.3203	0.03	1	554.3221	-3.15	$^{0,2}X_2$	H	+2Li
644.3466	0.04	1	644.3464	0.30	$^{1,5}A_3$	-2H	+1Li
678.3766	0.03	1	678.3769	-0.41	Z_3	2H	+1Li
682.3810	0.05	1	682.3809	0.22	B_3	H	+2Li
684.3860	0.17	1	684.3851	1.37	Z_3	H	+2Li
698.3759	0.33	1	698.3757	0.25	C_3	-H	+2Li
700.3801	0.83	1	700.3799	0.25	Y_3	-H	+2Li

779.4136	0.33	1	779.4121	1.85	$^{0,3}A_4$	H	+1Li
779.4136	0.33	1	779.4157	-2.71	$^{1,3}X_2$	3H	0
782.4219	0.03	1	782.4243	-3.01	$^{1,4}X_3$	2H	+1Li
826.4496	0.05	1	826.4504	-1.01	$^{1,3}X_3$	2H	+1Li
826.4496	0.05	1	826.4504	-1.01	$^{1,3}X_0$	2H	+1Li
826.4496	0.05	1	826.4504	-1.01	$^{2,4}X_3$	2H	+1Li
896.4673	1.37	1	896.4673	-0.01	C_4		+1Li

Table S12. List of EED fragment ions of the doubly lithiated, permethylated, ^{18}O-labeled LNnT at *m/z* 459.7513.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
195.1202	0.27	1	195.1203	-0.64	$^{1,5}A_1$	-2H	+1Li
225.1309	0.33	1	225.1309	0.08	B_1		+1Li
227.1351	0.46	1	227.1351	-0.12	Z_1		+1Li
241.1258	0.48	1	241.1258	-0.01	C_1	-2H	+1Li
243.1415	0.85	1	243.1414	0.20	C_1		+1Li
245.1457	0.39	1	245.1457	0.08	Y_1		+1Li
249.1496	1.24	1	249.1496	-0.11	C_1	-H	+2Li
273.1406	1.78	1	273.1406	-0.04	$^{1,5}X_1$		+1Li
301.1719	0.33	1	301.1719	-0.04	$^{0,2}X_1$		+1Li
307.1801	0.18	1	307.1801	0.06	$^{0,2}X_1$	-H	+2Li
313.1834	1.87	1	313.1833	0.35	$^{3,5}A_2$		+1Li
325.6809	0.12	2	651.3624	-0.94	$^{1,5}A_3$	-2H	+2Li
326.6887	0.09	2	653.3781	-1.06	$^{1,5}A_3$		+2Li
340.6862	0.04	2	681.3730	-0.93	B_3		+2Li
341.6883	0.14	2	683.3772	-0.93	Z_3		+2Li
349.6916	0.13	2	699.3835	-0.56	C_3		+2Li
364.6912	0.48	2	729.3827	-0.45	$^{1,5}X_3$		+2Li
377.7046	0.08	2	755.4097	-0.76	$^{2,4}A_4$		+2Li
378.7068	0.10	2	757.4140	-0.60	$^{0,2}X_3$		+2Li
384.7124	0.77	2	769.4254	-0.82	$^{3,5}A_4$		+2Li
421.7256	0.55	2	843.4508	0.44	$^{0,4}X_3$	-2H	+2Li
421.7256	0.55	2	843.4508	0.44	$^{0,4}X_2$	-2H	+2Li
421.7256	0.55	2	843.4508	0.44	$^{0,4}X_1$	-2H	+2Li
421.7256	0.55	2	843.4508	0.44	$^{0,4}X_0$	-2H	+2Li
422.7329	0.48	2	845.4664	-0.75	$^{0,4}X_3$		+2Li
422.7329	0.48	2	845.4664	-0.75	$^{0,4}X_2$		+2Li
422.7329	0.48	2	845.4664	-0.75	$^{0,4}X_1$		+2Li
422.7329	0.48	2	845.4664	-0.75	$^{0,4}X_0$		+2Li
427.7309	0.53	2	855.4622	-0.50	$^{1,5}A_4$	-2H	+2Li
428.7388	1.31	2	857.4778	-0.31	$^{1,5}A_4$		+2Li
431.2351	1.31	1	431.2349	0.47	Z_2		+1Li
442.2624	0.86	1	442.2623	0.25	$^{1,5}A_2$		+1Li
447.2299	1.22	1	447.2298	0.17	Y_2	-2H	+1Li

449.2455	6.91	1	449.2455	0.11	Y_2		+1Li
455.2536	6.82	1	455.2536	-0.09	Y_2	-H	+2Li
464.2492	1.05	1	464.2490	0.37	B_2	H	0
470.2573	5.66	1	470.2572	0.17	B_2		+1Li
477.2406	4.79	1	477.2404	0.49	$^{1,5}X_2$		+1Li
478.2811	0.16	1	478.2810	0.12	B_2	H	+2Li
486.2522	1.57	1	486.2521	0.15	C_2	-2H	+1Li
488.2678	0.16	1	488.2678	0.04	C_2		+1Li
533.2667	0.11	1	533.2666	0.25	$^{1,4}X_2$	-2H	+1Li
543.2871	0.06	1	543.2861	1.80	$^{1,3}A_3$	-H	+1Li
543.2871	0.06	1	543.2861	1.80	$^{2,4}A_3$	-H	+1Li
544.2941	0.26	1	544.2939	0.31	$^{1,3}A_3$		+1Li
544.2941	0.26	1	544.2939	0.31	$^{2,4}A_3$		+1Li
546.2983	0.14	1	546.2982	0.09	$^{0,2}X_2$		+1Li
588.3203	0.04	1	588.3202	0.19	$^{1,4}A_3$		+1Li
590.3246	0.16	1	590.3244	0.29	$^{0,3}X_2$		+1Li
600.3201	0.06	1	600.3202	-0.08	$^{2,5}A_3$	-2H	+1Li
612.3203	0.04	1	612.3226	-3.71	$^{0,2}A_3$	H	0
614.3253	0.05	1	614.3268	-2.50	$^{2,4}X_2$	H	0
644.3466	0.75	1	644.3464	0.30	$^{1,5}A_3$	-2H	+1Li
676.3613	1.85	1	676.3612	0.16	Z_3		+1Li
690.3520	0.86	1	690.3519	0.11	C_3	-2H	+1Li
692.3571	0.40	1	692.3561	1.43	Y_3	-2H	+1Li
694.3721	0.11	1	694.3718	0.42	Y_3		+1Li
698.3759	0.15	1	698.3757	0.25	C_3	-H	+2Li
700.3805	0.11	1	700.3799	0.77	Y_3	-H	+2Li
722.3670	1.21	1	722.3667	0.41	$^{1,5}X_3$		+1Li
728.3750	0.07	1	728.3749	0.15	$^{1,5}X_3$	-H	+2Li
747.3882	0.04	1	747.3859	3.02	$^{2,4}A_4$	-H	+1Li
750.3978	0.05	1	750.3980	-0.26	$^{0,2}X_3$		+1Li
762.4092	0.03	1	762.4094	-0.34	$^{3,5}A_4$		+1Li
777.3973	0.04	1	777.3965	1.02	$^{0,3}A_4$	-H	+1Li
777.3973	0.04	1	777.4000	-3.55	$^{1,3}X_2$	H	0
779.4142	0.02	1	779.4121	2.63	$^{0,3}A_4$	H	+1Li
838.4506	0.17	1	838.4504	0.20	$^{0,4}X_3$		+1Li
838.4506	0.17	1	838.4504	0.20	$^{0,4}X_2$		+1Li
838.4506	0.17	1	838.4504	0.20	$^{0,4}X_1$		+1Li
838.4506	0.17	1	838.4504	0.20	$^{0,4}X_0$		+1Li
896.4685	0.26	1	896.4673	1.35	C_4		+1Li

Table S13. List of EED fragment ions of the singly lithiated, permethylated, ^{18}O-labeled LNnT at *m/z* 912.4872.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
225.1309	0.06	1	225.1309	0.08	B_1		+1Li
227.1351	0.08	1	227.1351	-0.12	Z_1		+1Li
243.1415	0.23	1	243.1414	0.20	C_1		+1Li
245.1457	0.11	1	245.1457	0.08	Y_1		+1Li
273.1408	0.25	1	273.1406	0.74	$^{1,5}X_1$		+1Li
299.1678	0.08	1	299.1676	0.47	$^{2,4}A_2$		+1Li
313.1835	0.26	1	313.1833	0.64	$^{3,5}A_2$		+1Li
382.2051	0.05	1	382.2048	0.91	$^{1,4}A_2$	-2H	+1Li
430.2285	0.03	1	430.2271	3.26	Z_2	-H	+1Li
431.2352	1.07	1	431.2349	0.68	Z_2		+1Li
440.2478	0.07	1	440.2466	2.66	$^{1,5}A_2$	-2H	+1Li
442.2627	0.59	1	442.2623	0.94	$^{1,5}A_2$		+1Li
447.2301	1.18	1	447.2298	0.64	Y_2	-2H	+1Li
449.2458	7.60	1	449.2455	0.72	Y_2		+1Li
464.2493	0.08	1	464.2490	0.56	B_2	H	0
470.2575	2.58	1	470.2572	0.62	B_2		+1Li
477.2407	1.87	1	477.2404	0.68	$^{1,5}X_2$		+1Li
486.2523	1.31	1	486.2521	0.34	C_2	-2H	+1Li
487.2605	0.31	1	487.2599	1.13	C_2	-H	+1Li
488.2682	0.09	1	488.2678	0.85	C_2		+1Li
544.2942	0.19	1	544.2939	0.43	$^{1,3}A_3$		+1Li
544.2942	0.19	1	544.2939	0.43	$^{2,4}A_3$		+1Li
546.2985	0.05	1	546.2982	0.54	$^{0,2}X_2$		+1Li
590.3245	0.07	1	590.3244	0.19	$^{0,3}X_2$		+1Li
600.3206	0.02	1	600.3202	0.73	$^{2,5}A_3$	-2H	+1Li
614.3252	0.03	1	614.3268	-2.70	$^{2,4}X_2$	H	0
644.3465	0.65	1	644.3464	0.12	$^{1,5}A_3$	-2H	+1Li
645.3562	0.06	1	645.3542	3.03	$^{1,5}A_3$	-H	+1Li
676.3616	1.66	1	676.3612	0.52	Z_3		+1Li
678.3787	0.03	1	678.3769	2.73	Z_3	2H	+1Li
690.3518	0.83	1	690.3519	-0.16	C_3	-2H	+1Li
692.3569	0.11	1	692.3561	1.08	Y_3	-2H	+1Li

722.3667	1.38	1	722.3667	-0.02	$^{1,5}X_3$		+1Li
750.3981	0.04	1	750.3980	0.07	$^{0,2}X_3$		+1Li
762.4094	0.45	1	762.4094	-0.02	$^{3,5}A_4$		+1Li
804.4198	0.02	1	804.4200	-0.21	$^{2,5}A_4$	-2H	+1Li
836.4353	0.50	1	836.4348	0.60	$^{0,4}X_3$	-2H	+1Li
836.4353	0.50	1	836.4348	0.60	$^{0,4}X_2$	-2H	+1Li
836.4353	0.50	1	836.4348	0.60	$^{0,4}X_1$	-2H	+1Li
836.4353	0.50	1	836.4348	0.60	$^{0,4}X_0$	-2H	+1Li
838.4501	0.43	1	838.4504	-0.45	$^{0,4}X_3$		+1Li
838.4501	0.43	1	838.4504	-0.45	$^{0,4}X_2$		+1Li
838.4501	0.43	1	838.4504	-0.45	$^{0,4}X_1$		+1Li
838.4501	0.43	1	838.4504	-0.45	$^{0,4}X_0$		+1Li
848.4468	0.21	1	848.4462	0.66	$^{1,5}A_4$	-2H	+1Li
850.4614	0.70	1	850.4619	-0.52	$^{1,5}A_4$		+1Li

Table S14. List of EED fragment ions of the singly cesiated, permethylated, ^{18}O-labeled LNnT at *m/z* 1038.3767.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
262.9919	0.02	1	262.9917	0.75	$^{1,3}A_2$	H	+1Cs
292.9785	0.03	1	292.9785	0.10	$^{0,2}A_1$	-2H	+1Cs
351.0206	0.02	1	351.0203	0.74	B_1		+1Cs
353.0247	0.24	1	353.0246	0.30	Z_1		+1Cs
367.0153	0.27	1	367.0153	0.12	C_1	-2H	+1Cs
369.0310	0.35	1	369.0309	0.29	C_1		+1Cs
399.0302	0.09	1	399.0301	0.38	$^{1,5}X_1$		+1Cs
438.0649	0.01	1	438.0649	-0.03	$^{3,5}A_2$	-H	+1Cs
439.0729	0.08	1	439.0728	0.35	$^{3,5}A_2$		+1Cs
464.2491	0.09	1	464.2490	0.17	B_2	H	0
557.1244	1.52	1	557.1244	0.05	Z_2		+1Cs
566.1366	0.05	1	566.1361	0.92	$^{1,5}A_2$	-2H	+1Cs
568.1517	0.14	1	568.1517	-0.11	$^{1,5}A_2$		+1Cs
573.1197	0.92	1	573.1193	0.75	Y_2	-2H	+1Cs
575.1350	0.08	1	575.1349	0.16	Y_2		+1Cs
596.1468	0.18	1	596.1467	0.20	B_2		+1Cs
597.1548	0.05	1	597.1545	0.49	B_2	H	+1Cs
603.1298	1.09	1	603.1298	0.00	$^{1,5}X_2$		+1Cs
612.1415	2.27	1	612.1416	-0.15	C_2	-2H	+1Cs
613.1520	0.06	1	613.1494	4.21	C_2	-H	+1Cs
670.1834	0.15	1	670.1834	0.00	$^{1,3}A_3$		+1Cs
670.1834	0.15	1	670.1834	0.00	$^{2,4}A_3$		+1Cs
687.1753	0.04	1	687.1748	0.73	$^{2,5}X_2$	-H	+1Cs
716.2138	0.09	1	716.2139	-0.09	$^{0,3}X_2$		+1Cs
746.2248	0.03	1	746.2245	0.41	$^{2,4}X_2$		+1Cs
770.2358	0.43	1	770.2358	-0.12	$^{1,5}A_3$	-2H	+1Cs
802.2505	1.98	1	802.2507	-0.23	Z_3		+1Cs
816.2412	1.85	1	816.2413	-0.19	C_3	-2H	+1Cs
818.2466	0.08	1	818.2456	1.23	Y_3	-2H	+1Cs
848.2560	1.28	1	848.2562	-0.22	$^{1,5}X_3$		+1Cs
874.2831	0.04	1	874.2832	-0.14	$^{2,4}A_4$		+1Cs
876.2875	0.04	1	876.2875	0.00	$^{0,2}X_3$		+1Cs
887.2917	0.08	1	887.2911	0.71	$^{3,5}A_4$	-H	+1Cs

888.2989	0.49	1	888.2989	0.00	$^{3,5}A_4$		+1Cs
904.2831	0.02	1	904.2823	0.78	$^{1,4}X_3$	-2H	+1Cs
962.3251	0.30	1	962.3242	0.86	$^{0,4}X_3$	-2H	+1Cs
962.3251	0.30	1	962.3242	0.86	$^{0,4}X_2$	-2H	+1Cs
962.3251	0.30	1	962.3242	0.86	$^{0,4}X_1$	-2H	+1Cs
962.3251	0.30	1	962.3242	0.86	$^{0,4}X_0$	-2H	+1Cs
964.3399	0.88	1	964.3399	0.00	$^{0,4}X_3$		+1Cs
964.3399	0.88	1	964.3399	0.00	$^{0,4}X_2$		+1Cs
964.3399	0.88	1	964.3399	0.00	$^{0,4}X_1$		+1Cs
964.3399	0.88	1	964.3399	0.00	$^{0,4}X_0$		+1Cs
974.3354	0.23	1	974.3357	-0.28	$^{1,5}A_4$	-2H	+1Cs
976.3526	0.33	1	976.3513	1.31	$^{1,5}A_4$		+1Cs

Table S15. List of EED fragment ions of the singly lithiated, permethylated, and ^{18}O-Labeled Sialyl Lewis X at *m/z* 1039.5505.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
211.1149	0.51	1	211.1152	-1.60	$C_{1\beta}$	-2H	+1Li
213.1305	0.37	1	213.1309	-1.85	$C_{1\beta}$		+1Li
236.1466	0.08	1	236.1469	-1.11	$^{3,5}A_{1\alpha}$	-2H	+1Li
238.1621	0.07	1	238.1625	-1.78	$^{3,5}A_{1\alpha}$		+1Li
252.1415	0.04	1	252.1418	-1.10	$^{0,3}A_{1\alpha}$	-2H	+1Li
280.1727	0.04	1	280.1731	-1.37	$^{2,5}A_{1\alpha}$	-2H	+1Li
308.1678	0.10	1	308.1680	-0.65	$^{1,3}A_{3}$	-2H	+1Li
310.1836	0.08	1	310.1836	-0.14	$^{1,3}A_{3}$		+1Li
340.1941	6.38	1	340.1942	-0.33	$^{1,3}A_{3}$	OCH_2	+1Li
376.1966	0.08	1	376.1966	-0.03	$B_{1\alpha}$	H	0
382.2048	0.53	1	382.2048	0.05	$B_{1\alpha}$		+1Li
383.2126	0.29	1	383.2126	-0.06	$B_{1\alpha}$	H	+1Li
400.2151	0.12	1	400.2153	-0.64	$C_{1\alpha}$		+1Li
400.2153	0.13	1	400.2153	-0.11	$C_{1\alpha}$		+1Li
442.2509	0.89	1	442.2509	-0.03	$Z_{1\alpha}$		+1Li
454.2259	0.04	1	454.2259	-0.04	$^{1,3}A_{2\alpha}$	-2H	+1Li
454.2259	0.04	1	454.2259	-0.04	$^{2,4}A_{2\alpha}$	-2H	+1Li
456.2416	0.48	1	456.2415	0.11	$^{1,3}A_{2\alpha}$		+1Li
456.2416	0.48	1	456.2415	0.11	$^{2,4}A_{2\alpha}$		+1Li
458.2459	1.43	1	458.2458	0.23	$Y_{1\alpha}$	-2H	+1Li
460.2614	0.07	1	460.2614	-0.09	$Y_{1\alpha}$		+1Li
488.2564	1.32	1	488.2563	0.10	$^{1,5}X_{1\alpha}$		+1Li
498.2522	0.04	1	498.2521	0.15	$^{1,4}A_{2\alpha}$	-2H	+1Li
500.2662	0.04	1	500.2678	-3.13	$^{1,4}A_{2\alpha}$		+1Li
512.2678	0.12	1	512.2678	0.09	$^{2,5}A_{2\alpha}$	-2H	+1Li
514.2831	0.05	1	514.2834	-0.68	$^{2,5}A_{2\alpha}$		+1Li
514.2834	0.05	1	514.2834	-0.08	$^{2,5}A_{2\alpha}$		+1Li
516.2875	0.06	1	516.2877	-0.38	$^{0,2}X_{1\alpha}$		+1Li
528.2629	0.06	1	528.2627	0.37	$^{0,2}A_{2\alpha}$	-2H	+1Li
530.2785	0.03	1	530.2783	0.32	$^{0,2}A_{2\alpha}$		+1Li
556.2943	0.30	1	556.2940	0.57	$^{1,5}A_{2\alpha}$	-2H	+1Li
556.2949	0.35	1	556.2940	1.67	$^{1,5}A_{2\alpha}$	-2H	+1Li

558.3097	0.18	1	558.3096	0.09	$^{1,5}A_{2\alpha}$		+1Li
586.3047	0.05	1	586.3046	0.19	$B_{2\alpha}$		+1Li
588.3201	0.05	1	588.3203	-0.17	$B_{2\alpha}$	2H	+1Li
602.2994	1.55	1	602.2995	-0.18	$C_{2\alpha}$	-2H	+1Li
604.3151	0.25	1	604.3151	-0.02	$C_{2\alpha}$		+1Li
616.3403	1.60	1	616.3401	0.29	$Z_{2\alpha}$	$-OCH_2$	+1Li
646.3507	0.72	1	646.3506	0.08	$Z_{2\alpha}$		+1Li
662.3461	1.04	1	662.3456	0.85	$Y_{2\alpha}$	-2H	+1Li
664.3612	3.43	1	664.3612	-0.02	$Y_{2\alpha}$		+1Li
674.3571	0.16	1	674.3570	0.16	$^{3,5}A_3$		+1Li
734.3666	0.14	1	734.3667	-0.15	$^{1,3}X_0$	-2H	+1Li
748.3827	0.42	1	748.3823	0.47	$^{0,2}X_{2\alpha}$		+1Li
750.3616	0.28	1	750.3616	-0.10	$^{1,5}X_{2\alpha}$		+1Li
806.3880	0.02	1	806.3879	0.17	$^{3,5}X_{2\alpha}$	-2H	+1Li
833.4352	0.68	1	833.4351	0.06	$Z_{1\beta}$		+1Li
851.4455	0.06	1	851.4457	-0.23	$Y_{1\beta}$		+1Li
877.4607	0.10	1	877.4613	-0.71	$^{0,4}X_{2\alpha}$		+1Li
879.4410	0.41	1	879.4406	0.40	$^{1,5}X_{1\beta}$		+1Li
907.4715	0.06	1	907.4719	-0.42	$^{0,2}X_{1\beta}$		+1Li
907.4715	0.06	1	907.4719	-0.42	$^{1,4}X_{1\beta}$		+1Li
919.4715	0.04	1	919.4719	-0.45	$^{0,3}X_{1\alpha}$	-2H	+1Li
923.4664	0.04	1	923.4668	-0.48	$^{2,5}X_{1\beta}$		+1Li
935.4673	0.26	1	935.4669	0.47	$^{3,5}X_{1\alpha}$	-2H	+1Li
936.4752	0.09	1	936.4747	0.59	$^{3,5}X_{1\alpha}$	-H	+1Li
961.4863	0.02	1	961.4849	1.51	$^{3,5}X_{1\beta}$	H	0
963.4983	0.51	1	963.4981	0.20	$^{0,4}X_{1\alpha}$	-2H	+1Li
963.4983	0.51	1	963.4981	0.20	$^{0,4}X_0$	-2H	+1Li
965.5131	3.17	1	965.5137	-0.64	$^{0,4}X_{1\alpha}$		+1Li
965.5131	3.17	1	965.5137	-0.64	$^{0,4}X_0$		+1Li
979.4938	0.18	1	979.4930	0.76	$^{1,3}X_{2\alpha}$	-2H	+1Li
981.5079	0.74	1	981.5087	-0.82	$^{1,3}X_{2\alpha}$		+1Li
993.5091	0.35	1	993.5087	0.44	$^{0,4}X_{1\beta}$	-2H	+1Li
995.5245	0.38	1	995.5243	0.17	$^{0,4}X_{1\beta}$		+1Li
1007.5229	1.47	1	1007.5232	-0.27	$^{0,3}X_{1\beta}/C_3$	NOC_3H_6	+1Li

Table S16. List of EED fragment ions of the singly lithiated, permethylated, and ^{18}O-Labeled Sialyl Lewis A at *m/z* 1039.5505.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
211.1154	0.09	1	211.1152	0.79	$C_{1\beta}$	-2H	+1Li
213.1309	0.05	1	213.1309	0.09	$C_{1\beta}$		+1Li
238.1628	0.06	1	238.1625	1.17	$^{3,5}A_{1\alpha}$		+1Li
283.1729	0.03	1	283.1727	0.60	$^{3,5}A_{3}$		+1Li
340.1945	2.08	1	340.1942	0.81	$^{1,3}X_{2\alpha}/B_{2\alpha}$	CH_4	+1Li
376.1970	0.10	1	376.1966	1.02	$B_{1\alpha}$	H	0
382.2051	0.93	1	382.2048	0.85	$B_{1\alpha}$		+1Li
383.2129	0.29	1	383.2126	0.73	$B_{1\alpha}$	H	+1Li
400.2154	0.13	1	400.2153	0.12	$C_{1\alpha}$		+1Li
400.2157	0.14	1	400.2153	0.89	$C_{1\alpha}$		+1Li
436.2429	0.13	1	436.2427	0.39	$Z_{1\alpha}$	H	0
442.2512	1.40	1	442.2509	0.66	$Z_{1\alpha}$		+1Li
454.2263	0.04	1	454.2259	0.84	$^{1,3}A_{2\alpha}$	-2H	+1Li
454.2263	0.04	1	454.2259	0.84	$^{2,4}A_{2\alpha}$	-2H	+1Li
456.2418	0.22	1	456.2415	0.51	$^{1,3}A_{2\alpha}$		+1Li
456.2418	0.22	1	456.2415	0.51	$^{2,4}A_{2\alpha}$		+1Li
458.2461	0.15	1	458.2458	0.63	$Y_{1\alpha}$	-2H	+1Li
460.2618	0.11	1	460.2614	0.77	$Y_{1\alpha}$		+1Li
488.2566	0.83	1	488.2563	0.48	$^{1,5}X_{1\alpha}$		+1Li
498.2521	0.06	1	498.2521	-0.03	$^{1,4}A_{2\alpha}$	-2H	+1Li
502.2835	0.07	1	502.2834	0.17	$^{1,4}A_{2\alpha}$	2H	+1Li
512.2682	0.08	1	512.2678	0.80	$^{2,5}A_{2\alpha}$	-2H	+1Li
514.2835	0.08	1	514.2834	0.15	$^{2,5}A_{2\alpha}$		+1Li
516.2879	0.04	1	516.2877	0.45	$^{0,2}X_{1\alpha}$		+1Li
528.2634	0.12	1	528.2627	1.41	$^{0,2}A_{2\alpha}$	-2H	+1Li
530.2785	0.12	1	530.2783	0.32	$^{0,2}A_{2\alpha}$		+1Li
546.2979	0.08	1	546.2982	-0.58	$^{1,4}X_{1\alpha}$		+1Li
556.2938	0.18	1	556.2940	-0.31	$^{1,5}A_{2\alpha}$	-2H	+1Li
586.3042	0.06	1	586.3046	-0.64	$B_{2\alpha}$		+1Li
602.2994	4.90	1	602.2995	-0.18	$C_{2\alpha}$	-2H	+1Li
604.3150	0.80	1	604.3151	-0.22	$C_{2\alpha}$		+1Li
616.3400	0.90	1	616.3401	-0.16	$Z_{2\alpha}/^{0,4}X_{1\beta}$	CH_2	+1Li

646.3504	0.74	1	646.3506	-0.40	$Z_{2\alpha}$		+1Li
662.3459	1.12	1	662.3456	0.48	$Y_{2\alpha}$	-2H	+1Li
664.3611	5.28	1	664.3612	-0.20	$Y_{2\alpha}$		+1Li
701.3682	0.03	1	701.3679	0.51	$^{1,3}A_3$		+1Li
748.3827	0.80	1	748.3823	0.47	$^{0,2}X_{2\alpha}$		+1Li
750.3612	0.16	1	750.3616	-0.59	$^{1,5}X_{2\alpha}$		+1Li
833.4347	0.56	1	833.4351	-0.53	$Z_{1\beta}$		+1Li
849.4290	0.07	1	849.4301	-1.21	$Y_{1\beta}$	-2H	+1Li
851.4444	0.07	1	851.4457	-1.52	$Y_{1\beta}$		+1Li
877.4607	0.28	1	877.4613	-0.71	$^{0,4}X_{2\alpha}$		+1Li
879.4393	0.68	1	879.4406	-1.54	$^{1,5}X_{1\beta}$		+1Li
907.4709	0.06	1	907.4719	-1.09	$^{0,2}X_{1\beta}$		+1Li
907.4709	0.06	1	907.4719	-1.09	$^{1,4}X_{1\beta}$		+1Li
935.4658	0.21	1	935.4669	-1.09	$^{3,5}X_{1\alpha}$	-2H	+1Li
935.4656	0.21	1	935.4669	-1.36	$^{3,5}X_{1\alpha}$	-2H	+1Li
995.5232	0.24	1	995.5243	-1.12	$^{0,4}X_{1\beta}$		+1Li
963.4971	0.32	1	963.4981	-1.06	$^{0,4}X_{1\alpha}$	-2H	+1Li
963.4971	0.32	1	963.4981	-1.06	$^{0,4}X_0$	-2H	+1Li
965.5125	3.41	1	965.5137	-1.28	$^{0,4}X_{1\alpha}$		+1Li
965.5125	3.41	1	965.5137	-1.28	$^{0,4}X_0$		+1Li
979.4927	0.10	1	979.4930	-0.36	$^{1,3}X_{2\alpha}$	-2H	+1Li
981.5071	0.27	1	981.5087	-1.63	$^{1,3}X_{2\alpha}$		+1Li
993.5083	0.39	1	993.5087	-0.36	$^{0,4}X_{1\beta}$	-2H	+1Li
996.5299	0.20	1	996.5321	-2.23	$^{0,4}X_{1\beta}$	H	+1Li

Table S17. List of EED fragment ions of the singly lithiated, permethylated, $(Man)_5(GlcNAc)_2$ at *m/z* 1563.8808.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
511.2839	0.18	1	511.2838	0.28	Z_2		+1Li
557.2892	0.40	1	557.2892	-0.13	$^{1,5}X_2$		+1Li
649.3261	0.35	1	649.3254	1.15	$C_{2\alpha}$	-2H	+1Li
721.3830	0.27	1	721.3829	0.15	$^{3,5}A_3$		+1Li
877.4734	0.06	1	877.4727	0.75	$^{0,4}X_2$		+1Li
919.4834	0.26	1	919.4833	0.12	$Z_{3\alpha}$		+1Li
935.4790	0.13	1	935.4782	0.86	$Y_{3\alpha}$	-2H	+1Li
965.4889	0.82	1	965.4888	0.11	$^{1,5}X_{3\alpha}$		+1Li
1011.5204	0.18	1	1011.5194	0.98	$^{1,5}A_3$	-2H	+1Li
1013.5353	0.39	1	1013.5350	0.23	$^{1,5}A_3$		+1Li
1057.5247	7.37	1	1057.5249	-0.22	C_3	-2H	+1Li
1059.5440	0.57	1	1059.5405	3.21	C_3		+1Li
1129.5825	0.21	1	1129.5824	0.10	$^{3,5}A_4$		+1Li
1225.6111	0.08	1	1225.6147	-2.98	$^{1,4}X_2$	-2H	+1Li
1225.6111	0.08	1	1225.6147	-2.98	$^{1,4}X_{3\alpha}$	-2H	+1Li
1258.6613	0.20	1	1258.6614	-0.11	$^{1,5}A_4$		+1Li
1283.6578	0.62	1	1283.6566	0.96	$^{0,4}X_{3\alpha}$	-2H	+1Li
1286.6846	0.06	1	1286.6801	3.49	$^{0,4}X_{3\alpha}$	H	+1Li
1302.6519	2.15	1	1302.6512	0.48	C_4	-2H	+1Li
1305.6699	0.10	1	1305.6747	-3.67	C_4	H	+1Li
1327.6828	1.32	1	1327.6829	-0.10	$Z_{3\beta}$		+1Li
1327.6828	1.32	1	1327.6829	-0.10	$Z_{4\alpha'}$		+1Li
1327.6828	1.32	1	1327.6829	-0.10	$Z_{4\alpha''}$		+1Li
1343.6781	1.06	1	1343.6777	0.28	$Y_{3\beta}$	-2H	+1Li
1343.6781	1.06	1	1343.6777	0.28	$Y_{4\alpha'}$	-2H	+1Li
1343.6781	1.06	1	1343.6777	0.28	$Y_{4\alpha''}$	-2H	+1Li
1373.6878	3.31	1	1373.6884	-0.45	$^{1,5}X_{3\beta}$		+1Li
1373.6878	3.31	1	1373.6884	-0.45	$^{1,5}X_{4\alpha'}$		+1Li
1373.6878	3.31	1	1373.6884	-0.45	$^{1,5}X_{4\alpha''}$		+1Li

1429.7178	0.11	1	1429.7146	2.23	$^{1,4}X_{3\beta}$	-2H	+1Li
1429.7178	0.11	1	1429.7146	2.23	$^{1,4}X_{4\alpha'}$	-2H	+1Li
1429.7178	0.11	1	1429.7146	2.23	$^{1,4}X_{4\alpha''}$	-2H	+1Li
1459.7259	0.13	1	1459.7251	0.59	$^{3,5}X_{3\beta}$	-2H	+1Li
1459.7259	0.13	1	1459.7251	0.59	$^{3,5}X_{4\alpha'}$	-2H	+1Li
1459.7259	0.13	1	1459.7251	0.59	$^{3,5}X_{4\alpha''}$	-2H	+1Li
1462.7482	0.05	1	1462.7485	-0.27	$^{3,5}X_{3\beta}$	H	+1Li
1462.7482	0.05	1	1462.7485	-0.27	$^{3,5}X_{4\alpha'}$	H	+1Li
1462.7482	0.05	1	1462.7485	-0.27	$^{3,5}X_{4\alpha''}$	H	+1Li
1473.7420	0.10	1	1473.7407	0.84	$^{1,3}X_{3\beta}$	-2H	+1Li
1473.7420	0.10	1	1473.7407	0.84	$^{1,3}X_{4\alpha'}$	-2H	+1Li
1473.7420	0.10	1	1473.7407	0.84	$^{1,3}X_{4\alpha''}$	-2H	+1Li
1473.7420	0.10	1	1473.7407	0.84	$^{2,4}X_{3\beta}$	-2H	+1Li
1473.7420	0.10	1	1473.7407	0.84	$^{2,4}X_{4\alpha'}$	-2H	+1Li
1473.7420	0.10	1	1473.7407	0.84	$^{2,4}X_{4\alpha''}$	-2H	+1Li
1488.7648	0.60	1	1488.7643	0.33	$^{0,4}X_{0}$	-H	+1Li
1488.7648	0.60	1	1488.7643	0.33	$^{0,4}X_{1}$	-H	+1Li
1488.7648	0.60	1	1488.7643	0.33	$^{0,4}X_{3\beta}$	-H	+1Li
1488.7648	0.60	1	1488.7643	0.33	$^{0,4}X_{4\alpha'}$	-H	+1Li
1488.7648	0.60	1	1488.7643	0.33	$^{0,4}X_{4\alpha''}$	-H	+1Li
1489.7729	0.17	1	1489.7721	0.57	$^{0,4}X_{0}$		+1Li
1489.7729	0.17	1	1489.7721	0.57	$^{0,4}X_{1}$		+1Li
1489.7729	0.17	1	1489.7721	0.57	$^{0,4}X_{3\beta}$		+1Li
1489.7729	0.17	1	1489.7721	0.57	$^{0,4}X_{4\alpha'}$		+1Li
1489.7729	0.17	1	1489.7721	0.57	$^{0,4}X_{4\alpha''}$		+1Li
1501.7736	0.60	1	1501.7721	0.98	$^{1,5}A_{5}$	-2H	+1Li
1531.7841	2.04	1	1531.7826	0.95	B_{5}		+1Li
1547.7793	0.72	1	1547.7776	1.11	C_{5}	-2H	+1Li

Table S18. List of EED fragment ions of the doubly lithiated, permethylated, $(Man)_5(GlcNAc)_2$ at *m/z* 785.4121.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
243.1414	0.16	1	243.1414	-0.17	$C_{1\alpha'}$		+1Li
243.1414	0.16	1	243.1414	-0.17	$C_{1\alpha''}$		+1Li
243.1414	0.16	1	243.1414	-0.17	$C_{1\beta}$		+1Li
249.1496	0.89	1	249.1496	-0.11	$C_{1\alpha'}$	-H	+2Li
249.1496	0.89	1	249.1496	-0.11	$C_{1\alpha''}$	-H	+2Li
249.1496	0.89	1	249.1496	-0.11	$C_{1\beta}$	-H	+2Li
266.1574	0.32	1	266.1574	-0.04	Z_1		+1Li
284.1680	0.52	1	284.1680	0.07	Y_1		+1Li
285.1520	0.33	1	285.1520	-0.04	$^{0,4}A_{2\alpha}$		+1Li
290.1762	0.50	1	290.1761	0.17	Y_1	-H	+2Li
291.1602	0.60	1	291.1602	-0.04	$^{0,4}A_{2\alpha}$	-H	+2Li
312.1629	0.53	1	312.1629	-0.04	$^{1,5}X_1$		+1Li
313.1833	0.21	1	313.1833	-0.04	$^{3,5}A_{2\alpha}$		+1Li
509.2682	0.04	2	1018.5354	0.96	$^{1,5}A_3$	-2H	+2Li
511.2837	0.79	1	511.2838	-0.14	Z_2		+1Li
513.2994	0.06	1	513.2994	-0.07	Z_2	2H	+1Li
527.2787	0.19	1	527.2787	0.03	Y_2	-2H	+1Li
529.2944	0.23	1	529.2943	0.09	Y_2		+1Li
532.2708	0.30	2	1064.5409	0.69	C_3	-2H	+2Li
533.2783	0.16	2	1066.5565	0.09	C_3		+2Li
535.3025	0.45	1	535.3025	-0.02	Y_2	-H	+2Li
557.2893	0.80	1	557.2892	0.09	$^{1,5}X_2$		+1Li
559.2935	0.04	1	559.2936	-0.19	$^{2,5}A_{2\alpha}$	-2H	+1Li
568.2991	0.09	2	1136.5984	-0.24	$^{3,5}A_4$		+2Li
585.3203	0.04	1	585.3205	-0.33	$^{0,2}X_2$		+1Li
603.3206	0.27	1	603.3199	1.24	$^{1,5}A_{2\alpha}$	-2H	+1Li
605.3356	0.35	1	605.3355	0.08	$^{1,5}A_{2\alpha}$		+1Li
611.3170	0.04	2	1222.6300	3.27	$^{1,4}X_2$	2H	0

611.3170	0.04	2	1222.6300	3.27	$^{1,4}X_{3\alpha}$	2H	0
616.3130	0.04	2	1232.6307	-3.86	$^{1,4}X_{2}$	-2H	+2Li
616.3130	0.04	2	1232.6307	-3.86	$^{1,4}X_{3\alpha}$	-2H	+2Li
632.8385	0.28	2	1265.6774	-0.31	$^{1,5}A_{4}$		+2Li
645.3360	0.43	2	1290.6726	-0.47	$^{0,4}X_{3\alpha}$	-2H	+2Li
646.3431	0.19	2	1292.6882	-1.62	$^{0,4}X_{3\alpha}$		+2Li
646.8357	0.19	2	1293.6722	-0.68	B_{4}		+2Li
649.3260	0.54	1	649.3254	0.96	$C_{2\alpha}$	-2H	+1Li
654.8331	1.09	2	1309.6672	-0.74	C_{4}	-2H	+2Li
656.3437	0.28	2	1312.6907	-2.54	C_{4}	H	+2Li
657.3493	0.77	1	657.3492	0.17	$C_{2\alpha}$	-H	+2Li
666.8454	0.06	2	1333.6910	-0.19	$Z_{3\beta}$	-H	+2Li
666.8454	0.06	2	1333.6910	-0.19	$Z_{4\alpha'}$	-H	+2Li
666.8454	0.06	2	1333.6910	-0.19	$Z_{4\alpha''}$	-H	+2Li
667.3492	0.90	2	1334.6989	-0.38	$Z_{3\beta}$		+2Li
667.3492	0.90	2	1334.6989	-0.38	$Z_{4\alpha'}$		+2Li
667.3492	0.90	2	1334.6989	-0.38	$Z_{4\alpha''}$		+2Li
675.3466	0.99	2	1350.6937	-0.36	$Y_{3\beta}$	-2H	+2Li
675.3466	0.99	2	1350.6937	-0.36	$Y_{4\alpha'}$	-2H	+2Li
675.3466	0.99	2	1350.6937	-0.36	$Y_{4\alpha''}$	-2H	+2Li
676.3556	0.16	2	1352.7094	1.34	$Y_{3\beta}$		+2Li
676.3556	0.16	2	1352.7094	1.34	$Y_{4\alpha'}$		+2Li
676.3556	0.16	2	1352.7094	1.34	$Y_{4\alpha''}$		+2Li
683.3443	0.10	2	1366.6849	2.69	$^{3,5}A_{5}$	-H	0
689.3450	0.09	2	1378.6887	0.89	$^{1,5}X_{3\beta}$	-2H	+2Li
689.3450	0.09	2	1378.6887	0.89	$^{1,5}X_{4\alpha'}$	-2H	+2Li
689.3450	0.09	2	1378.6887	0.89	$^{1,5}X_{4\alpha''}$	-2H	+2Li
690.3520	3.49	2	1380.7043	-0.28	$^{1,5}X_{3\beta}$		+2Li
690.3520	3.49	2	1380.7043	-0.28	$^{1,5}X_{4\alpha'}$		+2Li
690.3520	3.49	2	1380.7043	-0.28	$^{1,5}X_{4\alpha''}$		+2Li
693.3515	0.76	1	693.3516	-0.11	$^{0,4}A_{3}$		+1Li
699.3599	2.57	1	699.3597	0.25	$^{0,4}A_{3}$	-H	+2Li
704.3677	0.11	2	1408.7356	-0.19	$^{0,2}X_{3\beta}$		+2Li
704.3677	0.11	2	1408.7356	-0.19	$^{0,2}X_{4\alpha'}$		+2Li
704.3677	0.11	2	1408.7356	-0.19	$^{0,2}X_{4\alpha''}$		+2Li
711.3588	0.04	2	1422.7148	1.97	$^{2,5}X_{3\beta}$	-2H	+2Li

711.3588	0.04	2	1422.7148	1.97	$^{2,5}X_{4\alpha'}$	-2H	+2Li
711.3588	0.04	2	1422.7148	1.97	$^{2,5}X_{4\alpha''}$	-2H	+2Li
712.3655	0.03	2	1424.7305	0.33	$^{2,5}X_{3\beta}$		+2Li
712.3655	0.03	2	1424.7305	0.33	$^{2,5}X_{4\alpha'}$		+2Li
712.3655	0.03	2	1424.7305	0.33	$^{2,5}X_{4\alpha''}$		+2Li
718.3653	0.11	2	1436.7306	0.00	$^{1,4}X_{3\beta}$	-2H	+2Li
718.3653	0.11	2	1436.7306	0.00	$^{1,4}X_{4\alpha'}$	-2H	+2Li
718.3653	0.11	2	1436.7306	0.00	$^{1,4}X_{4\alpha''}$	-2H	+2Li
721.3829	0.42	1	721.3829	-0.02	$^{3,5}A_{3}$		+1Li
731.3744	0.03	2	1462.7485	0.15	$^{3,5}X_{3\beta}$	H	+1Li
731.3744	0.03	2	1462.7485	0.15	$^{3,5}X_{4\alpha'}$	H	+1Li
731.3744	0.03	2	1462.7485	0.15	$^{3,5}X_{4\alpha''}$	H	+1Li
733.3720	0.08	2	1466.7411	2.00	$^{3,5}X_{3\beta}$	-2H	+2Li
733.3720	0.08	2	1466.7411	2.00	$^{3,5}X_{4\alpha'}$	-2H	+2Li
733.3720	0.08	2	1466.7411	2.00	$^{3,5}X_{4\alpha''}$	-2H	+2Li
740.3801	0.07	2	1480.7567	2.39	$^{1,3}X_{3\beta}$	-2H	+2Li
740.3801	0.07	2	1480.7567	2.39	$^{1,3}X_{4\alpha'}$	-2H	+2Li
740.3801	0.07	2	1480.7567	2.39	$^{1,3}X_{4\alpha''}$	-2H	+2Li
740.3801	0.07	2	1480.7567	2.39	$^{2,4}X_{3\beta}$	-2H	+2Li
740.3801	0.07	2	1480.7567	2.39	$^{2,4}X_{4\alpha'}$	-2H	+2Li
740.3801	0.07	2	1480.7567	2.39	$^{2,4}X_{4\alpha''}$	-2H	+2Li
742.3924	0.05	2	1484.7880	-2.17	$^{1,3}X_{3\beta}$	2H	+2Li
742.3924	0.05	2	1484.7880	-2.17	$^{1,3}X_{4\alpha'}$	2H	+2Li
742.3924	0.05	2	1484.7880	-2.17	$^{1,3}X_{4\alpha''}$	2H	+2Li
742.3924	0.05	2	1484.7880	-2.17	$^{2,4}X_{3\beta}$	2H	+2Li
742.3924	0.05	2	1484.7880	-2.17	$^{2,4}X_{4\alpha'}$	2H	+2Li
742.3924	0.05	2	1484.7880	-2.17	$^{2,4}X_{4\alpha''}$	2H	+2Li
747.3853	0.67	2	1494.7725	-1.22	$^{0,4}X_{0}$	-2H	+2Li
747.3853	0.67	2	1494.7725	-1.22	$^{0,4}X_{1}$	-2H	+2Li
747.3853	0.67	2	1494.7725	-1.22	$^{0,4}X_{3\beta}$	-2H	+2Li
747.3853	0.67	2	1494.7725	-1.22	$^{0,4}X_{4\alpha'}$	-2H	+2Li
747.3853	0.67	2	1494.7725	-1.22	$^{0,4}X_{4\alpha''}$	-2H	+2Li
748.3945	0.57	2	1496.7881	0.55	$^{0,4}X_{0}$		+2Li
748.3945	0.57	2	1496.7881	0.55	$^{0,4}X_{1}$		+2Li
748.3945	0.57	2	1496.7881	0.55	$^{0,4}X_{3\beta}$		+2Li
748.3945	0.57	2	1496.7881	0.55	$^{0,4}X_{4\alpha'}$		+2Li

748.3945	0.57	2	1496.7881	0.55	$^{0,4}X_{4\alpha''}$		+2Li
754.3942	0.82	2	1508.7881	0.24	$^{1,5}A_5$	-2H	+2Li
768.3908	0.08	2	1536.7830	-0.87	B_5	-2H	+2Li
769.3992	2.54	2	1538.7986	-0.17	B_5		+2Li
774.8938	0.09	2	1549.7932	-3.63	C_5		+1Li
777.9000	0.47	2	1555.8014	-0.87	C_5	-H	+2Li
875.4584	0.08	1	875.4571	1.48	$^{0,4}X_2$	-2H	+1Li
877.4730	0.24	1	877.4727	0.33	$^{0,4}X_2$		+1Li
919.4835	0.26	1	919.4833	0.25	$Z_{3\alpha}$		+1Li
935.4793	0.11	1	935.4782	1.19	$Y_{3\alpha}$	-2H	+1Li
937.4944	0.12	1	937.4938	0.57	$Y_{3\alpha}$		+1Li
943.5021	1.12	1	943.5020	0.05	$Y_{3\alpha}$	-H	+2Li
965.4887	0.97	1	965.4888	-0.08	$^{1,5}X_{3\alpha}$		+1Li
993.5194	0.06	1	993.5201	-0.69	$^{0,2}X_{3\alpha}$		+1Li
1011.5186	0.47	1	1011.5194	-0.77	$^{1,5}A_3$	-2H	+1Li
1013.5360	0.25	1	1013.5350	0.95	$^{1,5}A_3$		+1Li
1041.5301	0.07	1	1041.5299	0.22	B_3		+1Li
1057.5245	4.25	1	1057.5249	-0.33	C_3	-2H	+1Li
1060.5470	0.16	1	1060.5483	-1.29	C_3	H	+1Li
1065.5496	0.08	1	1065.5487	0.79	C_3	-H	+2Li
1129.5821	0.18	1	1129.5824	-0.23	$^{3,5}A_4$		+1Li
1150.5827	0.05	1	1150.5776	4.35	$^{0,3}A_4$	-2H	+2Li
1194.6096	0.05	1	1194.6039	4.80	$^{0,2}A_4$	-2H	+2Li
1194.6096	0.05	1	1194.6113	-1.44	$^{1,4}A_4$	H	0
1258.6611	0.06	1	1258.6614	-0.20	$^{1,5}A_4$		+1Li
1280.6680	0.04	1	1280.6719	-3.07	$^{0,4}X_{3\alpha}$	2H	0
1286.6556	1.12	1	1286.6563	-0.48	B_4		+1Li
1327.6827	0.26	1	1327.6829	-0.10	$Z_{3\beta}$		+1Li
1327.6827	0.26	1	1327.6829	-0.10	$Z_{4\alpha'}$		+1Li
1327.6827	0.26	1	1327.6829	-0.10	$Z_{4\alpha''}$		+1Li
1333.6925	0.07	1	1333.6910	1.09	$Z_{3\beta}$	-H	+2Li
1333.6925	0.07	1	1333.6910	1.09	$Z_{4\alpha'}$	-H	+2Li
1333.6925	0.07	1	1333.6910	1.09	$Z_{4\alpha''}$	-H	+2Li
1345.6930	0.05	1	1345.6934	-0.28	$Y_{3\beta}$		+1Li
1345.6930	0.05	1	1345.6934	-0.28	$Y_{4\alpha'}$		+1Li
1345.6930	0.05	1	1345.6934	-0.28	$Y_{4\alpha''}$		+1Li

1351.7010	2.58	1	1351.7015	-0.37	$Y_{3\beta}$	-H	+2Li
1351.7010	2.58	1	1351.7015	-0.37	$Y_{4\alpha'}$	-H	+2Li
1351.7010	2.58	1	1351.7015	-0.37	$Y_{4\alpha''}$	-H	+2Li
1373.6859	0.14	1	1373.6884	-1.79	$^{1,5}X_{3\beta}$		+1Li
1373.6859	0.14	1	1373.6884	-1.79	$^{1,5}X_{4\alpha'}$		+1Li
1373.6859	0.14	1	1373.6884	-1.79	$^{1,5}X_{4\alpha''}$		+1Li
1401.7191	0.26	1	1401.7196	-0.36	$^{0,2}X_{3\beta}$		+1Li
1401.7191	0.26	1	1401.7196	-0.36	$^{0,2}X_{4\alpha'}$		+1Li
1401.7191	0.26	1	1401.7196	-0.36	$^{0,2}X_{4\alpha''}$		+1Li
1407.7267	0.10	1	1407.7278	-0.79	$^{0,2}X_{3\beta}$	-H	+2Li
1407.7267	0.10	1	1407.7278	-0.79	$^{0,2}X_{4\alpha'}$	-H	+2Li
1407.7267	0.10	1	1407.7278	-0.79	$^{0,2}X_{4\alpha''}$	-H	+2Li
1417.7104	0.10	1	1417.7145	-2.85	$^{2,5}X_{3\beta}$		+1Li
1417.7104	0.10	1	1417.7145	-2.85	$^{2,5}X_{4\alpha'}$		+1Li
1417.7104	0.10	1	1417.7145	-2.85	$^{2,5}X_{4\alpha''}$		+1Li
1428.7188	0.07	1	1428.7217	-2.06	$^{0,2}A_5$	H	0
1428.7188	0.07	1	1428.7217	-2.06	$^{1,3}X_0$	H	0
1428.7188	0.07	1	1428.7217	-2.06	$^{1,3}X_1$	H	0
1433.7425	0.05	1	1433.7458	-2.32	$^{1,4}X_{3\beta}$	2H	+1Li
1433.7425	0.05	1	1433.7458	-2.32	$^{1,4}X_{4\alpha'}$	2H	+1Li
1433.7425	0.05	1	1433.7458	-2.32	$^{1,4}X_{4\alpha''}$	2H	+1Li
1463.7532	0.08	1	1463.7563	-2.19	$^{3,5}X_{3\beta}$	2H	+1Li
1463.7532	0.08	1	1463.7563	-2.19	$^{3,5}X_{4\alpha'}$	2H	+1Li
1463.7532	0.08	1	1463.7563	-2.19	$^{3,5}X_{4\alpha''}$	2H	+1Li
1495.7809	0.18	1	1495.7803	0.40	$^{0,4}X_0$	-H	+2Li
1495.7809	0.18	1	1495.7803	0.40	$^{0,4}X_1$	-H	+2Li
1495.7809	0.18	1	1495.7803	0.40	$^{0,4}X_{3\beta}$	-H	+2Li
1495.7809	0.18	1	1495.7803	0.40	$^{0,4}X_{4\alpha'}$	-H	+2Li
1495.7809	0.18	1	1495.7803	0.40	$^{0,4}X_{4\alpha''}$	-H	+2Li
1531.7831	0.04	1	1531.7826	0.31	B_5		+1Li
1537.7909	0.78	1	1537.7908	0.07	B_5	-H	+2Li
1539.8024	0.05	1	1539.8064	-2.64	B_5	H	+2Li
1547.7803	0.04	1	1547.7776	1.74	C_5	-2H	+1Li
1549.7945	0.10	1	1549.7932	0.86	C_5		+1Li
1555.8009	1.13	1	1555.8014	-0.32	C_5	-H	+2Li

Table S19. List of EED fragment ions of the singly cesiated, permethylated, and ^{18}O-Labeled Sialyl Lewis X at *m/z* 1165.4400.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
337.0047	0.06	1	337.0047	0.05	$C_{1\beta}$	-2H	+1Cs
362.0364	0.06	1	362.0363	0.25	$^{3,5}A_{1\alpha}$	-2H	+1Cs
376.1965	0.02	1	376.1966	-0.28	$B_{1\alpha}$	H	0
436.0731	0.02	1	436.0731	0.00	$^{1,3}A_{3}$		+1Cs
466.0837	4.96	1	466.0836	0.13	$^{1,3}A_{3}$	OCH2	+1Cs
508.0944	0.19	1	508.0942	0.30	$B_{1\alpha}$		+1Cs
509.1020	0.24	1	509.1021	-0.15	$B_{1\alpha}$	H	+1Cs
568.1403	0.62	1	568.1404	-0.05	$Z_{1\alpha}$		+1Cs
582.1309	0.09	1	582.1310	-0.16	$^{1,3}A_{2\alpha}$		+1Cs
582.1309	0.09	1	582.1310	-0.16	$^{2,4}A_{2\alpha}$		+1Cs
584.1353	0.12	1	584.1353	0.10	$Y_{1\alpha}$	-2H	+1Cs
614.1457	0.67	1	614.1458	-0.20	$^{1,5}X_{1\alpha}$		+1Cs
624.1413	0.03	1	624.1416	-0.44	$^{1,4}A_{2\alpha}$	-2H	+1Cs
638.1576	0.04	1	638.1572	0.57	$^{2,5}A_{2\alpha}$	-2H	+1Cs
640.1729	0.06	1	640.1729	0.05	$^{2,5}A_{2\alpha}$		+1Cs
654.1522	0.09	1	654.1521	0.14	$^{0,2}A_{2\alpha}$	-2H	+1Cs
656.1582	0.03	1	656.1564	2.74	$^{2,5}X_{1\alpha}$	-2H	+1Cs
658.1721	0.03	1	658.1721	0.09	$^{2,5}X_{1\alpha}$		+1Cs
682.1837	0.17	1	682.1835	0.40	$^{1,5}A_{2\alpha}$	-2H	+1Cs
684.1989	0.16	1	684.1991	-0.27	$^{1,5}A_{2\alpha}$		+1Cs
714.1976	0.03	1	714.1982	-0.98	$^{1,3}X_{1\alpha}$	-2H	+1Cs
714.1976	0.03	1	714.1982	-0.98	$^{2,4}X_{1\alpha}$	-2H	+1Cs
728.1886	2.44	1	728.1890	-0.46	$C_{2\alpha}$	-2H	+1Cs
730.2058	0.08	1	730.2046	1.67	$C_{2\alpha}$		+1Cs
742.2292	1.84	1	742.2296	-0.48	$Z_{2\alpha}$	$-OCH_2$	+1Cs
772.2403	0.60	1	772.2401	0.24	$Z_{2\alpha}$		+1Cs
788.2348	1.14	1	788.2350	-0.27	$Y_{2\alpha}$	-2H	+1Cs
790.2512	0.58	1	790.2507	0.70	$Y_{2\alpha}$		+1Cs
800.2462	0.10	1	800.2465	-0.31	$^{3,5}A_{3}$		+1Cs
827.4263	0.04	1	827.4269	-0.83	$Z_{1\beta}$	H	0
860.2560	0.21	1	860.2561	-0.18	$^{1,3}X_{0}$	-2H	+1Cs
876.2507	0.18	1	876.2511	-0.49	$^{1,5}X_{2\alpha}$		+1Cs

917.3135	0.17	1	917.3140	-0.58	$Z_{1\beta}/^{1,3}X_{2\alpha}$	CH_4	+1Cs
959.3237	0.50	1	959.3246	-0.89	$Z_{1\beta}$		+1Cs
975.3178	0.06	1	975.3195	-1.72	$Y_{1\beta}$	-2H	+1Cs
977.3353	0.05	1	977.3351	0.19	$Y_{1\beta}$		+1Cs
1003.3503	0.15	1	1003.3508	-0.49	$^{0,4}X_{2\alpha}$		+1Cs
1005.3306	0.65	1	1005.3301	0.55	$^{1,5}X_{1\beta}$		+1Cs
1033.3608	0.07	1	1033.3613	-0.47	$^{0,2}X_{1\beta}$		+1Cs
1033.3608	0.07	1	1033.3613	-0.47	$^{1,4}X_{1\beta}$		+1Cs
1089.3864	0.63	1	1089.3876	-1.09	$^{0,4}X_{1\alpha}$	-2H	+1Cs
1089.3864	0.63	1	1089.3876	-1.09	$^{0,4}X_{0}$	-2H	+1Cs
1091.4026	3.13	1	1091.4032	-0.56	$^{0,4}X_{1\alpha}$		+1Cs
1091.4026	3.13	1	1091.4032	-0.56	$^{0,4}X_{0}$		+1Cs
1105.3815	0.21	1	1105.3824	-0.91	$^{1,3}X_{2\alpha}$	-2H	+1Cs
1107.3975	0.81	1	1107.3982	-0.61	$^{1,3}X_{2\alpha}$		+1Cs
1119.3986	0.44	1	1119.3981	0.41	$^{0,4}X_{1\beta}$	-2H	+1Cs
1121.4147	0.33	1	1121.4138	0.82	$^{0,4}X_{1\beta}$		+1Cs
1133.4138	1.46	1	1133.4126	1.06	$^{0,3}X_{1\beta}/C_3$	NOC_3H_6	+1Cs

Table S20. List of EED fragment ions of the singly cesiated, permethylated, and ^{18}O-Labeled Sialyl Lewis A at *m/z* 1165.4400.

Exp. m/z (Da/e)	Relative Intensity (%)	charge state (z)	Theo. Mass	Error (ppm)	Fragment Types	Loss or Gain	number of metal adducts
337.0047	0.06	1	337.0047	0.05	$C_{1\beta}$	-2H	+1Cs
362.0357	0.06	1	362.0363	-1.69	$^{3,5}A_{1\alpha}$	-2H	+1Cs
376.1962	0.02	1	376.1966	-1.09	$B_{1\alpha}$	H	0
406.0619	0.02	1	406.0625	-1.58	$^{2,5}A_{1\alpha}$	-2H	+1Cs
409.0615	0.02	1	409.0622	-1.72	$^{3,5}A_{3}$		+1Cs
436.2422	0.03	1	436.2427	-1.22	$Z_{1\alpha}$	H	0
466.0832	2.04	1	466.0837	-1.01	$^{1,3}X_{2\alpha}/B_{2\alpha}$	CH_4	+1Cs
508.0949	0.44	1	508.0942	1.32	$B_{1\alpha}$		+1Cs
509.1018	0.20	1	509.1021	-0.51	$B_{1\alpha}$	H	+1Cs
524.0894	0.03	1	524.0891	0.52	$C_{1\alpha}$	-2H	+1Cs
526.1047	0.07	1	526.1048	-0.23	$C_{1\alpha}$		+1Cs
568.1401	0.79	1	568.1404	-0.48	$Z_{1\alpha}$		+1Cs
580.1159	0.02	1	580.1154	0.95	$^{1,3}A_{2\alpha}$	-2H	+1Cs
580.1159	0.02	1	580.1154	0.95	$^{2,4}A_{2\alpha}$	-2H	+1Cs
582.1309	0.08	1	582.1310	-0.16	$^{1,3}A_{2\alpha}$		+1Cs
582.1309	0.08	1	582.1310	-0.16	$^{2,4}A_{2\alpha}$		+1Cs
584.1356	0.14	1	584.1353	0.63	$Y_{1\alpha}$	-2H	+1Cs
614.1458	0.65	1	614.1458	0.00	$^{1,5}X_{1\alpha}$		+1Cs
624.1415	0.03	1	624.1416	-0.15	$^{1,4}A_{2\alpha}$	-2H	+1Cs
638.1578	0.05	1	638.1572	0.86	$^{2,5}A_{2\alpha}$	-2H	+1Cs
640.1730	0.05	1	640.1729	0.14	$^{2,5}A_{2\alpha}$		+1Cs
642.1767	0.04	1	642.1771	-0.67	$^{0,2}X_{1\alpha}$		+1Cs
654.1522	0.18	1	654.1521	0.14	$^{0,2}A_{2\alpha}$	-2H	+1Cs
656.1679	0.05	1	656.1678	0.19	$^{0,2}A_{2\alpha}$		+1Cs
670.1718	0.04	1	670.1720	-0.32	$^{1,4}X_{1\alpha}$	-2H	+1Cs
682.1839	0.12	1	682.1835	0.67	$^{1,5}A_{2\alpha}$	-2H	+1Cs
684.1991	0.07	1	684.1991	0.00	$^{1,5}A_{2\alpha}$		+1Cs
698.1784	0.24	1	698.1784	0.03	$B_{2\alpha}$	$-CH_2$	+1Cs
698.1784	0.24	1	698.1783	0.04	$C_{2\alpha}$	$-OCH_4$	+1Cs
714.1733	0.34	1	714.1733	-0.02	$C_{2\alpha}$	$-CH_4$	+1Cs
728.1889	6.29	1	728.1890	-0.04	$C_{2\alpha}$	-2H	+1Cs
730.2052	0.33	1	730.2046	0.84	$C_{2\alpha}$		+1Cs

742.2295	1.31	1	742.2296	-0.07	$Z_{2\alpha}$	$-OCH_2$	+1Cs
758.2247	0.28	1	758.2245	0.28	$Y_{2\alpha}$	$-OCH_4$	+1Cs
758.2247	0.28	1	758.2245	0.27	$Z_{2\alpha}$	$-CH_2$	+1Cs
772.2479	0.08	1	772.2515	-4.64	$Y_{2\alpha}/B_3$	CH_4	+1Cs
788.2360	0.93	1	788.2350	1.28	$Y_{2\alpha}$	-2H	+1Cs
790.2510	0.64	1	790.2507	0.39	$Y_{2\alpha}$		+1Cs
827.2574	0.07	1	827.2573	0.07	$^{1,3}A_3$		+1Cs
827.4271	0.03	1	827.4269	0.21	$Z_{1\beta}$	H	0
873.2873	0.03	1	873.2878	-0.56	$^{0,3}X_0$		+1Cs
874.2709	0.53	1	874.2718	-1.05	$^{0,2}X_{2\alpha}$		+1Cs
876.2507	0.17	1	876.2511	-0.49	$^{1,5}X_{2\alpha}$		+1Cs
959.3244	0.66	1	959.3246	-0.19	$Z_{1\beta}$		+1Cs
975.3205	0.04	1	975.3195	1.03	$Y_{1\beta}$	-2H	+1Cs
977.3354	0.04	1	977.3351	0.25	$Y_{1\beta}$		+1Cs
1003.3499	0.17	1	1003.3508	-0.85	$^{0,4}X_{2\alpha}$		+1Cs
1005.3301	0.76	1	1005.3301	0.00	$^{1,5}X_{1\beta}$		+1Cs
1031.3460	0.02	1	1031.3457	0.27	$^{0,2}X_{1\beta}$	-2H	+1Cs
1031.3460	0.02	1	1031.3457	0.27	$^{1,4}X_{1\beta}$	-2H	+1Cs
1033.3616	0.07	1	1033.3613	0.24	$^{0,2}X_{1\beta}$		+1Cs
1033.3616	0.07	1	1033.3613	0.24	$^{1,4}X_{1\beta}$		+1Cs
1045.3617	0.03	1	1045.3613	0.32	$^{0,3}X_{1\alpha}$	-2H	+1Cs
1047.3765	0.03	1	1047.3770	-0.52	$^{0,3}X_{1\alpha}$		+1Cs
1049.3550	0.02	1	1049.3562	-1.22	$^{2,5}X_{1\beta}$		+1Cs
1061.3580	0.26	1	1061.3563	1.64	$^{3,5}X_{1\alpha}$	-2H	+1Cs
1077.3873	0.02	1	1077.3876	-0.23	$^{0,3}X_{1\beta}$		+1Cs
1077.3873	0.02	1	1077.3876	-0.23	$^{1,3}X_{1\beta}$		+1Cs
1077.3873	0.02	1	1077.3876	-0.23	$^{2,4}X_{1\beta}$		+1Cs
1089.3878	0.49	1	1089.3876	0.25	$^{0,4}X_{1\alpha}$	-2H	+1Cs
1089.3878	0.49	1	1089.3876	0.25	$^{0,4}X_0$	-2H	+1Cs
1091.4034	3.12	1	1091.4032	0.22	$^{0,4}X_{1\alpha}$		+1Cs
1091.4034	3.12	1	1091.4032	0.22	$^{0,4}X_0$		+1Cs
1105.3827	0.18	1	1105.3824	0.19	$^{1,3}X_{2\alpha}$	-2H	+1Cs
1107.3980	0.85	1	1107.3982	-0.17	$^{1,3}X_{2\alpha}$		+1Cs
1119.3994	0.40	1	1119.3981	1.17	$^{0,4}X_{1\beta}$	-2H	+1Cs
1121.4154	0.18	1	1121.4138	1.47	$^{0,4}X_{1\beta}$		+1Cs
1122.4200	0.04	1	1122.4216	-1.37	$^{0,4}X_{1\beta}$	H	+1Cs