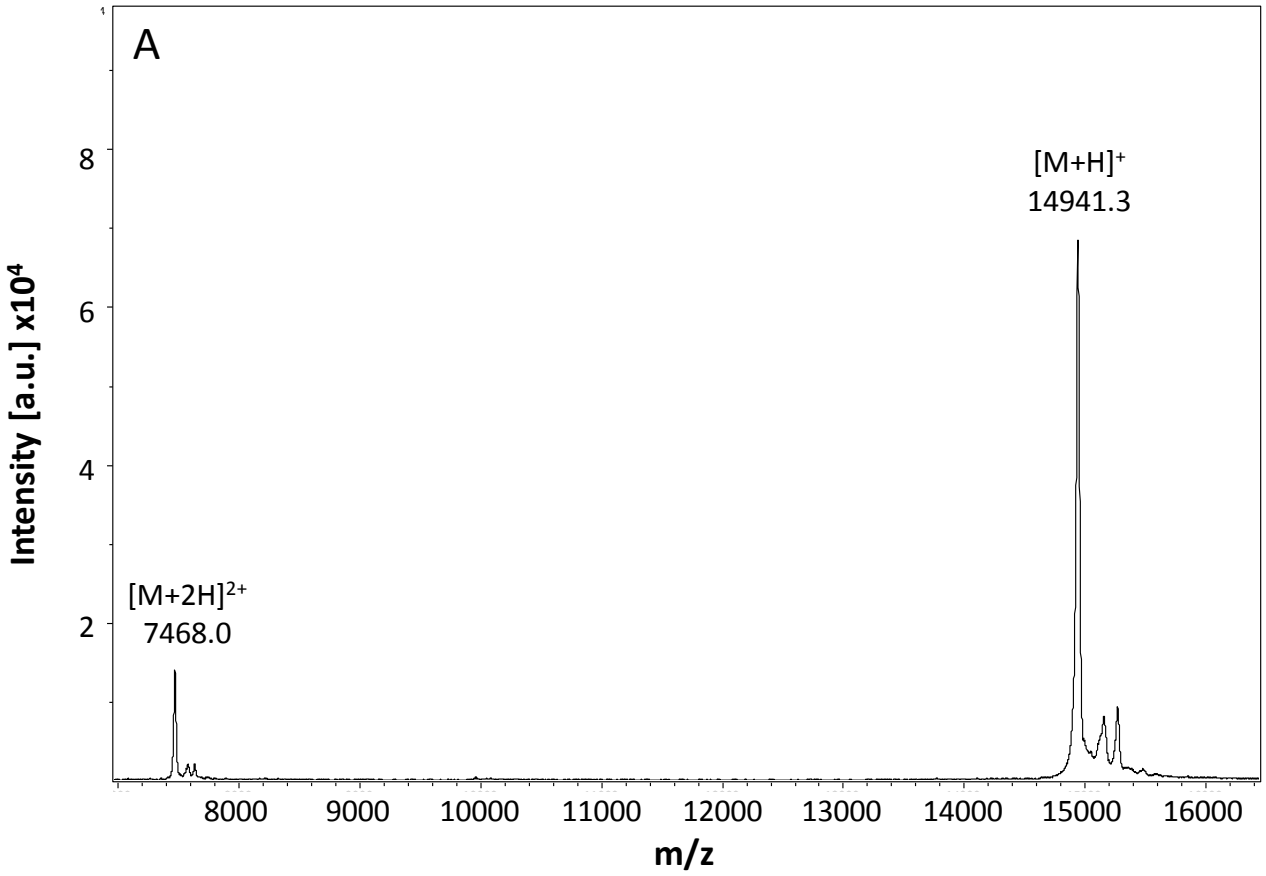
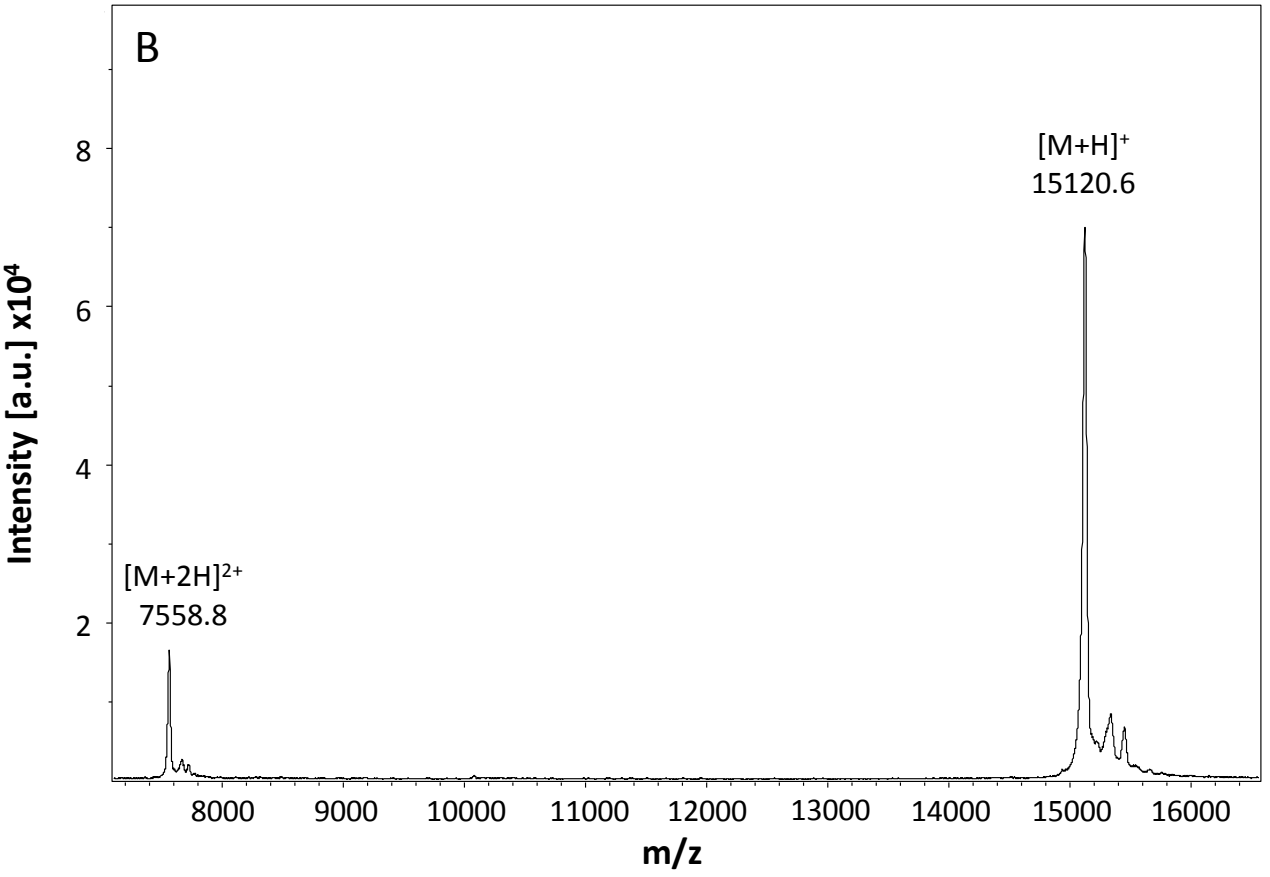




Supplemental Figure S1

Gal-7 mass determined by MALDI-TOF MS. Mass determination of Gal-7 (A) and ^{15}N-labelled Gal-7 (B) by MALDI-TOF measured on an Ultraflex™ TOFTOF I instrument (Bruker Daltonik) equipped with a nitrogen laser (20 Hz). Intact proteins prepared with the SA matrix were analyzed in the positive-ion linear mode using the following settings: ion acceleration voltage at 25.0 kV and first extraction plate at 23.2 kV. Expected molecular weights are ~14945 Da for ^{14}N and ~15146 Da for ^{15}N.

A

SNVPHKSSLPEGIRPGTVLRIRGLVPPNASRFHVNLLCGEEQGSDAALHFNPRLDTSEVVFNSKEQGSW
GREERGPGVPFQRGQPFEVLIIASDDGFKAVVGDAQYHHFRHRLPLARVRLVEVGGDVQLDSVRIF

Sequence	$[MH]^+$ calc	$[MH]^+$ exp
EQGSWGR	819.4	819.4
GPGVPFQR	857.5	857.5
HRLPLAR	862.5	862.5
GLVPPNASR	910.5	910.5
EQGSWGREER	1233.6	1233.6
LDTSEVVFNSK	1238.6	1238.6
AVVGDAQYHHFR	1399.7	1399.7
SSLPEGIRPGTVLR	1481.8	1481.8
LVEVGGDVQLDSVR	1485.8	1485.8
GQPFEVLIIASDDGFK	1735.9	1735.9
LDTSEVVFNSKEQGSWGREER	2453.2	2453.2
FHVNLLCGEEQGSDAALHFNPR	2454.2	2454.1
FHVNLLCGEEQGSDAALHFNPR*	2511.2	2511.2

*Carbamidomethyl at C

B

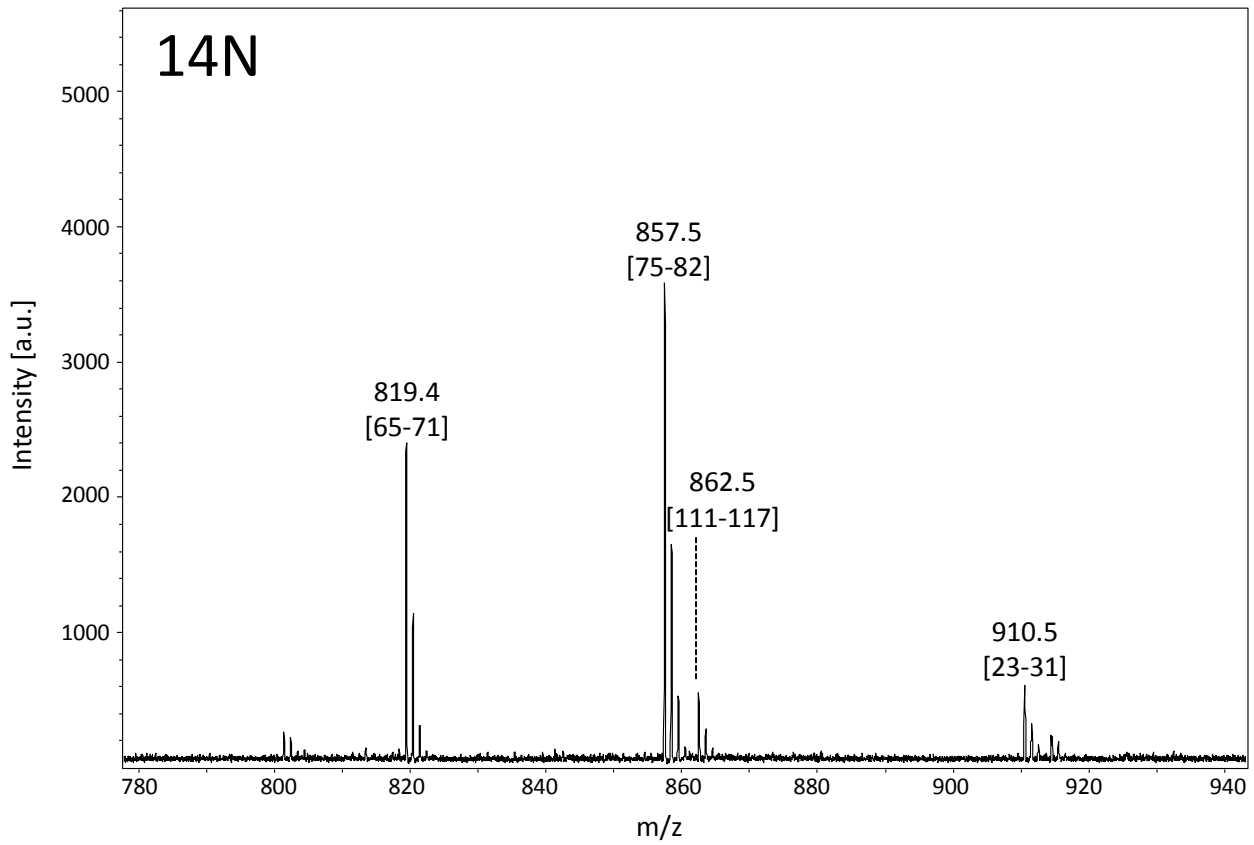
SNVPHKSSLPEGIRPGTVLRIRGLVPPNASRFHVNLLCGEEQGSDAALHFNPRLDTSEVVFNSKEQGSW
GREERGPGVPFQRGQPFEVLIIASDDGFKAVVGDAQYHHFRHRLPLARVRLVEVGGDVQLDSVRIF

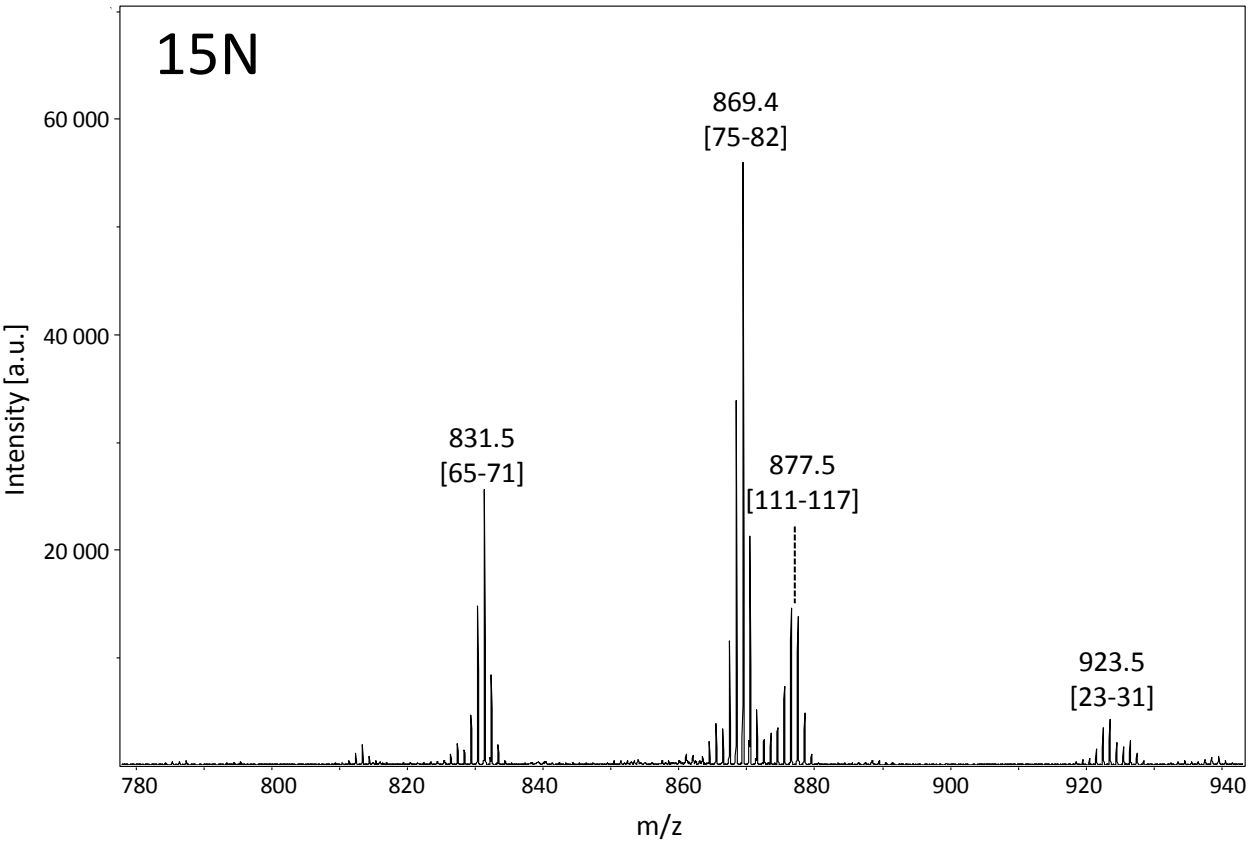
Sequence (# of nitrogens)	$[MH]^+$ calc	$[MH]^+$ exp
EQGSWGR (12)	831.3	831.4
GPGVPFQR (12)	869.4	869.4
HRLPLAR (15)	877.5	877.5
GLVPPNASR (13)	923.5	923.5
LDTSEVVFNSK (13)	1251.6	1251.6
AVVGDAQYHHFR (20)	1419.6	1419.7
SSLPEGIRPGTVLR (20)	1501.8	1501.9
SNVPHKSSLPEGIR (21)	1541.8	1541.6
GQPFEVLIIASDDGFK (18)	1753.8	1753.8
FHVNLLCGEEQGSDAALHFNPR (32)	2542.1	2542.1

*Carbamidomethyl at C

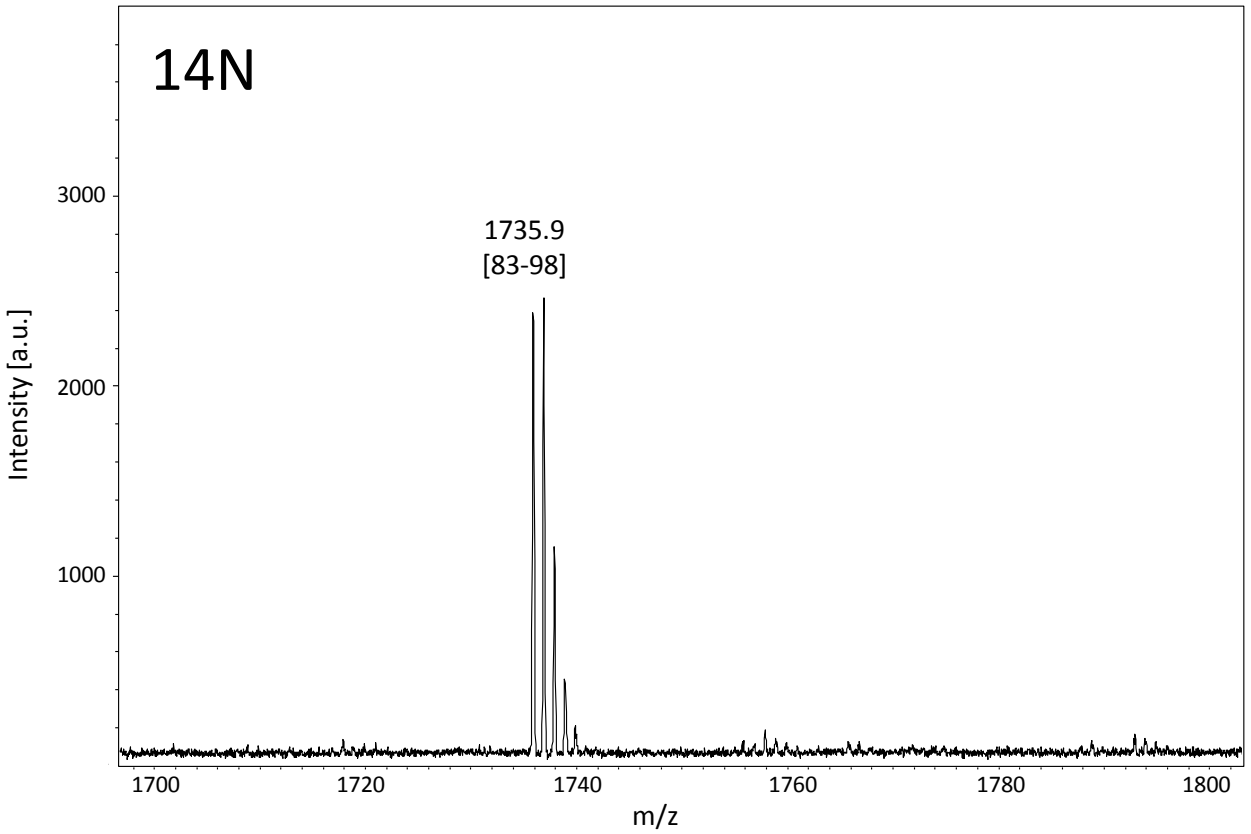
Peptide fingerprinting by MS. Peptide fingerprinting spectra were recorded in two positive-ion reflectron modes with ion acceleration voltage at 25.0 kV, reflector voltage at 26.3 kV and first extraction plate at 21.75 kV and 21.65 kV. Experimental information from up to 1000 individual laser shots was routinely accumulated. Calculated and experimentally determined peptide masses and the corresponding sequence alignment for Gal-7 (A) and ^{15}N-labeled Gal-7 (B). Sequence coverage is 91.1% for gal-7 and 83% for 15N-labelled galectin-7. Number of nitrogens in the peptide is given in brackets.

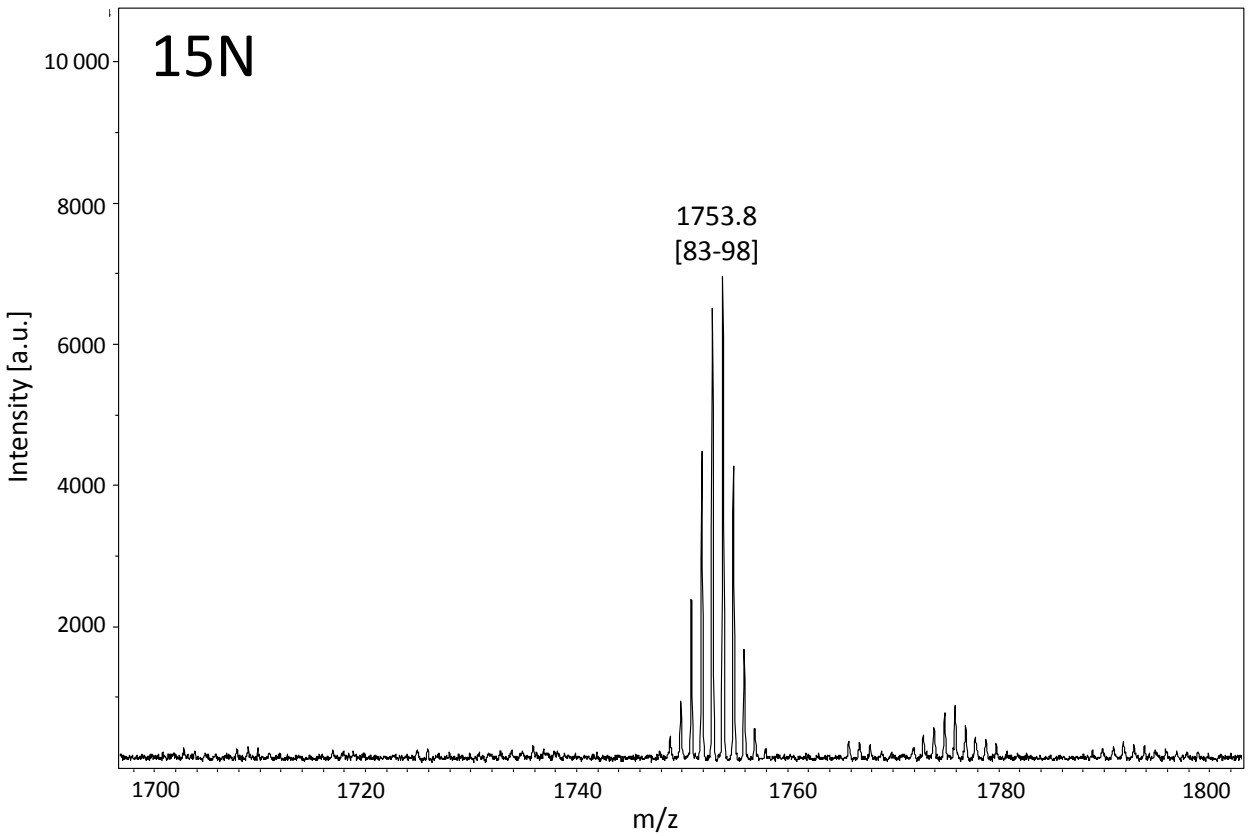
Supplemental Figure S2



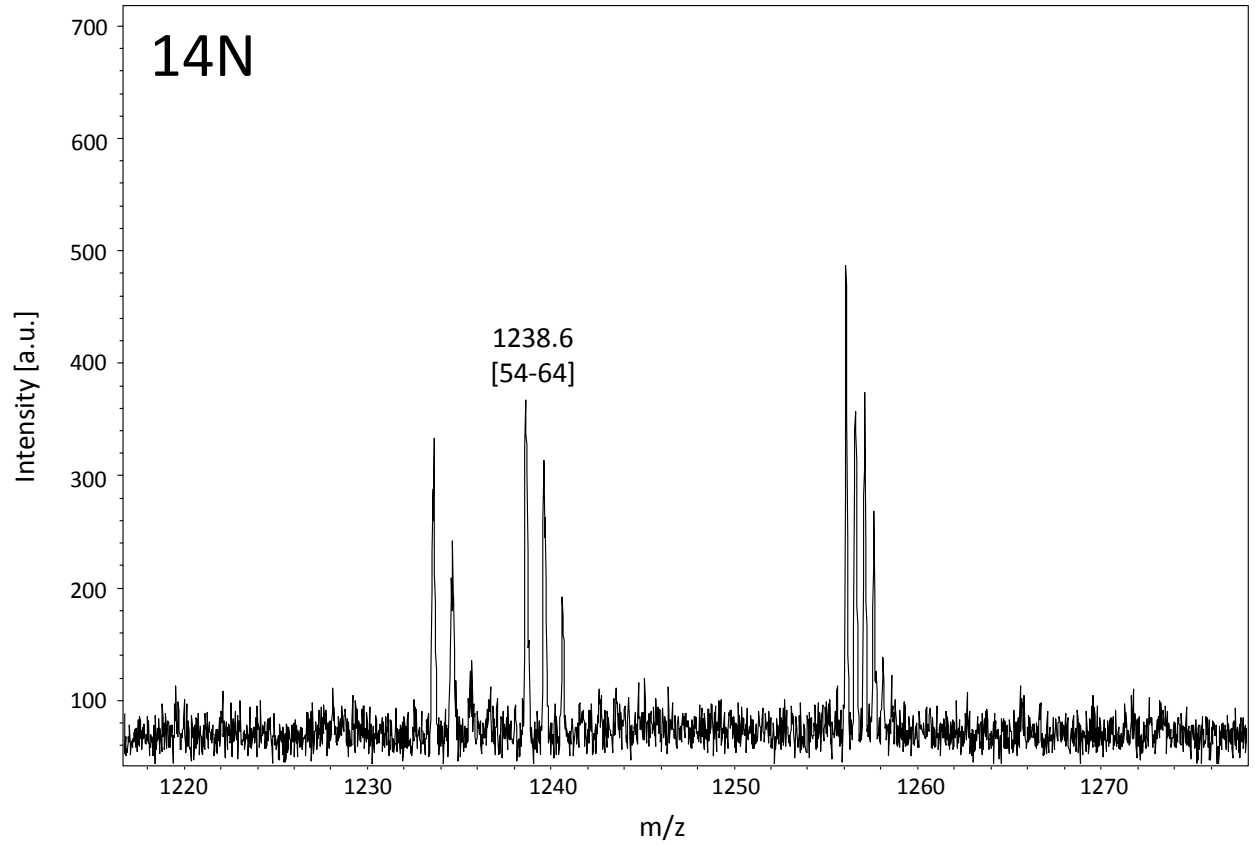


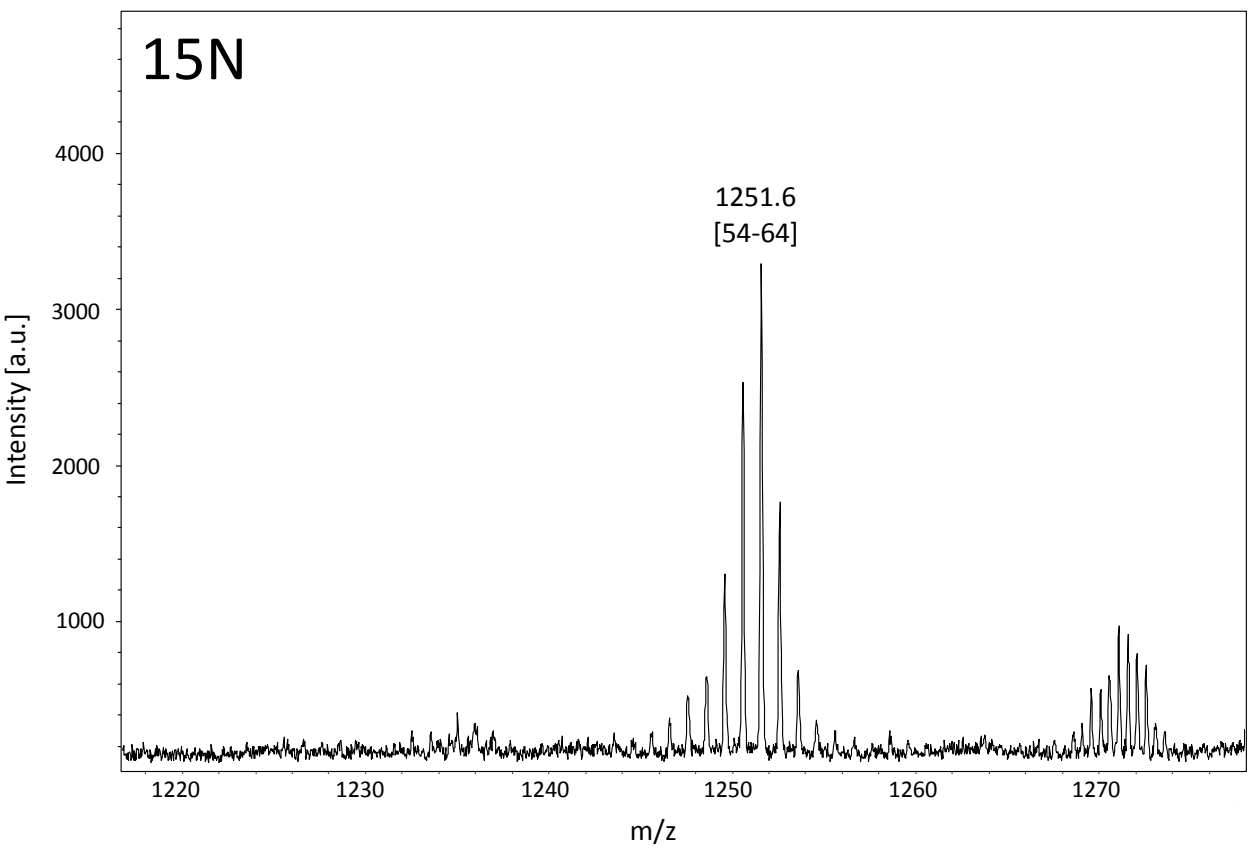
Supplemental Figure S3



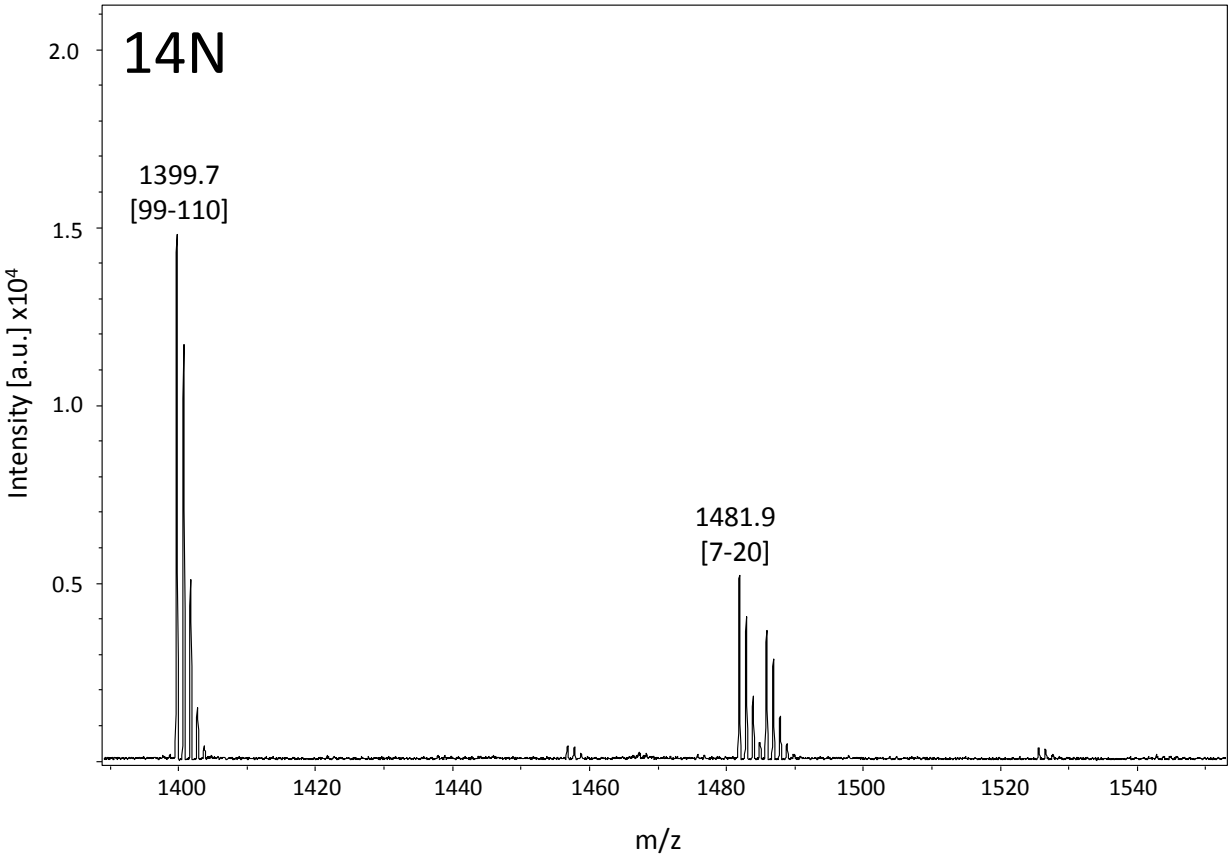


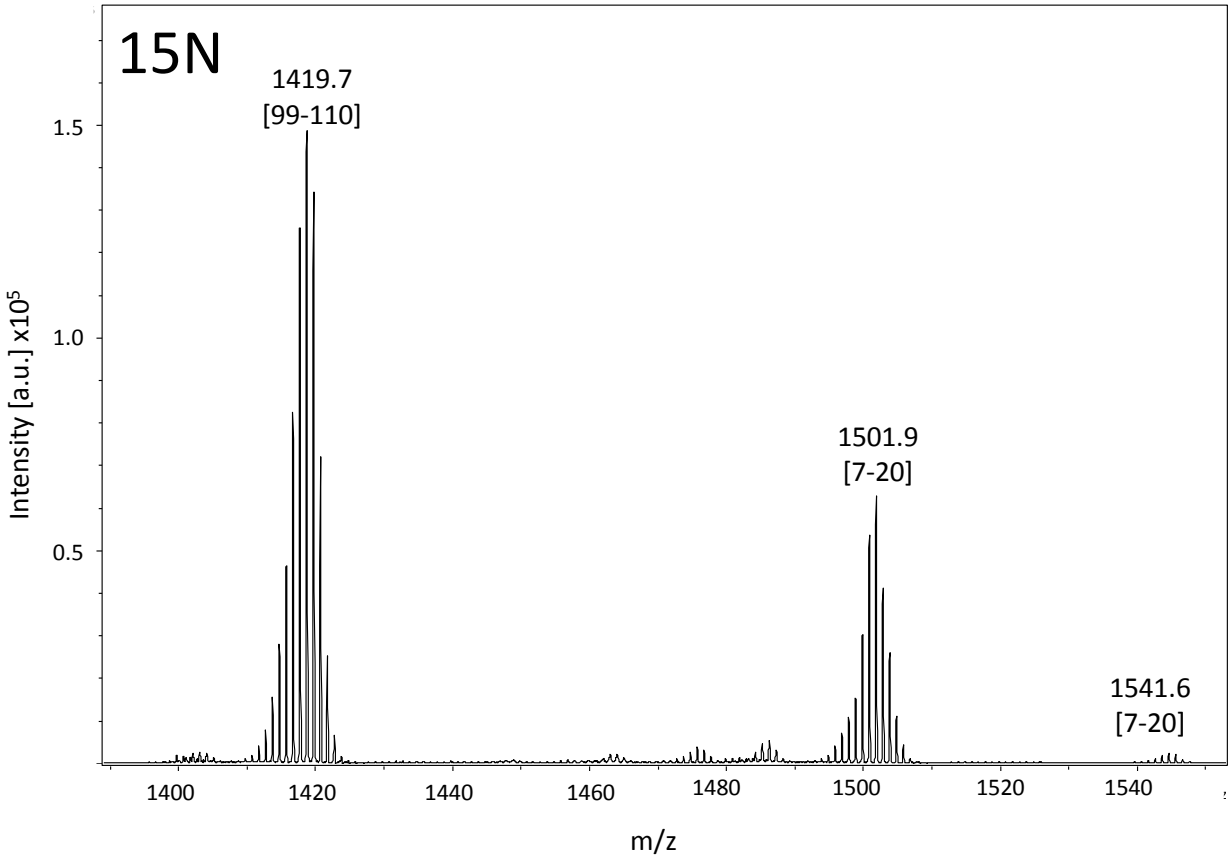
Supplemental Figure S3



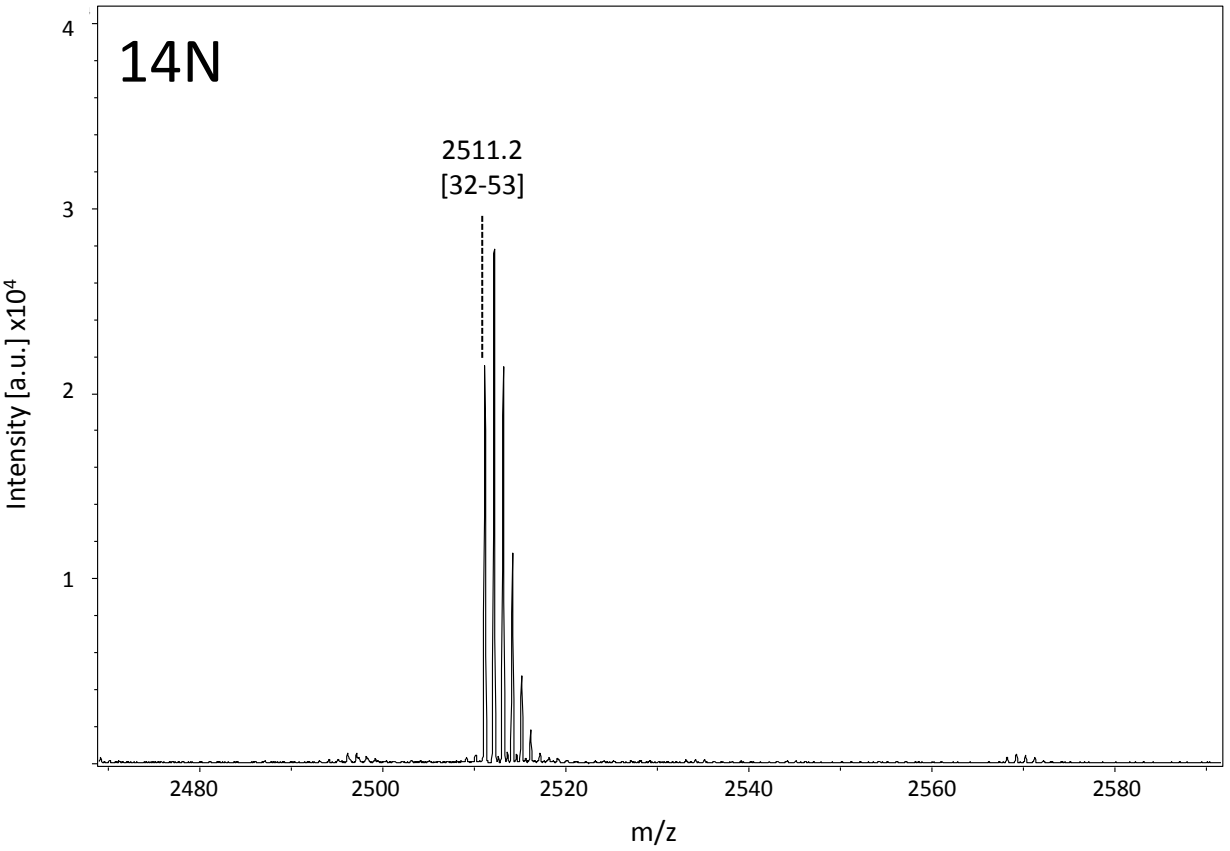


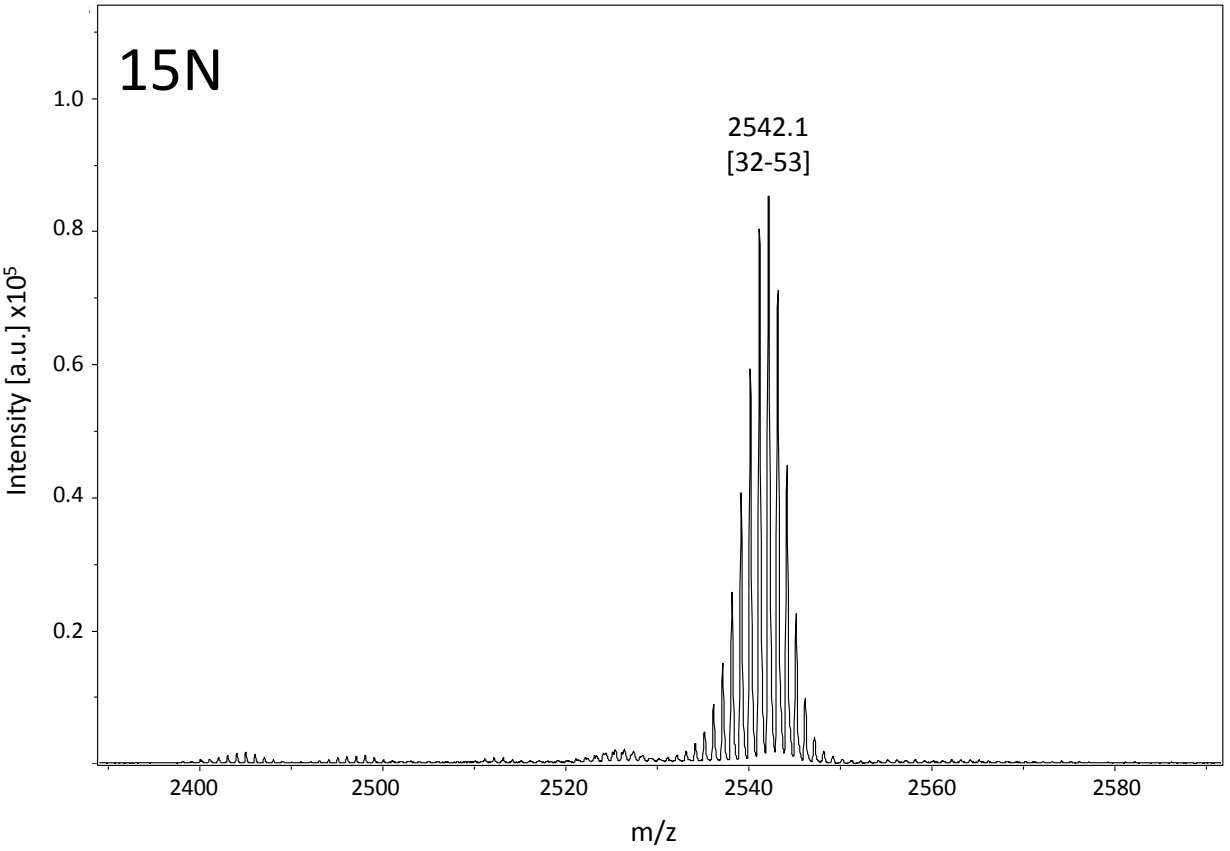
Supplemental Figure S3





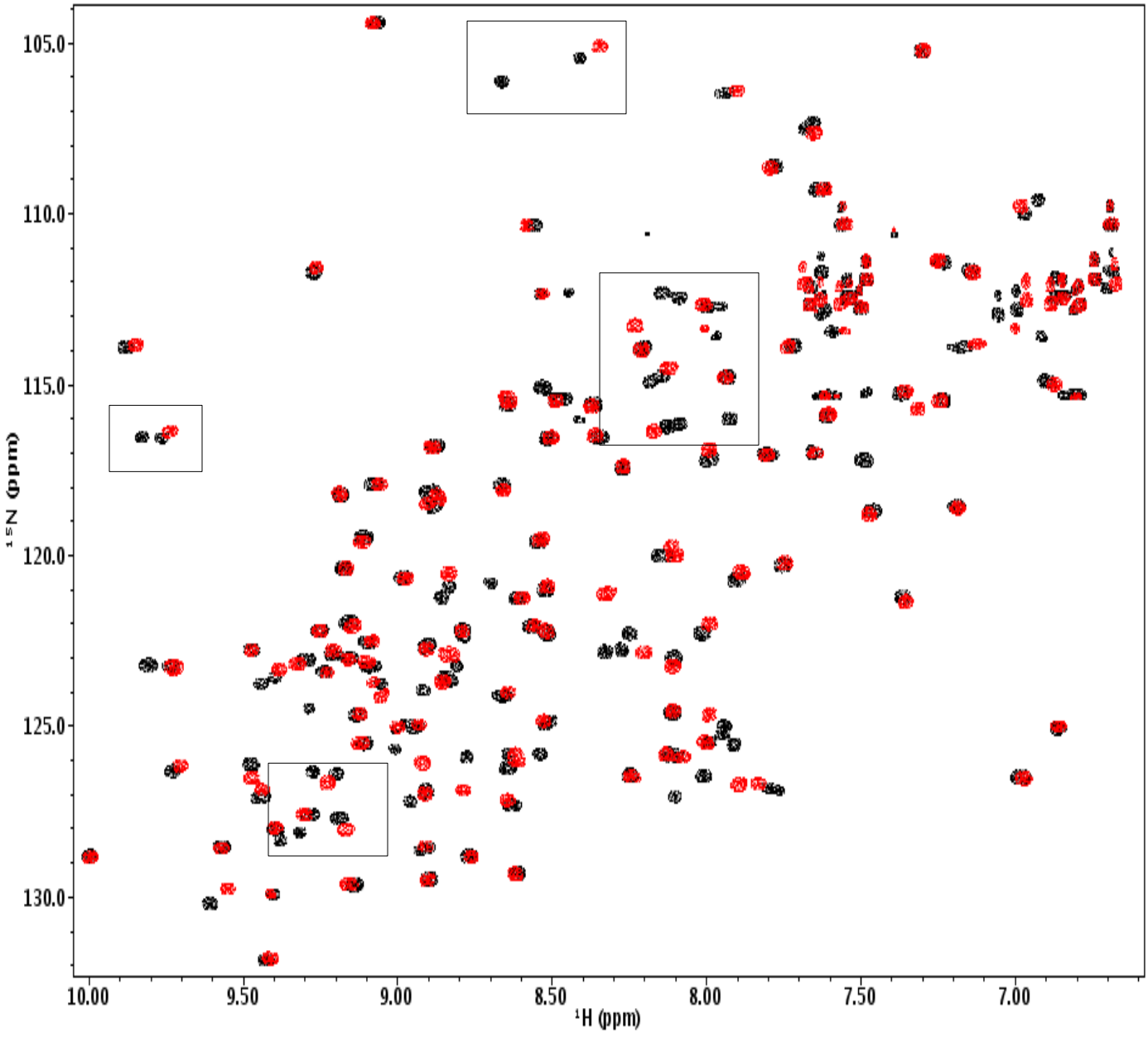
Supplemental Figure S3





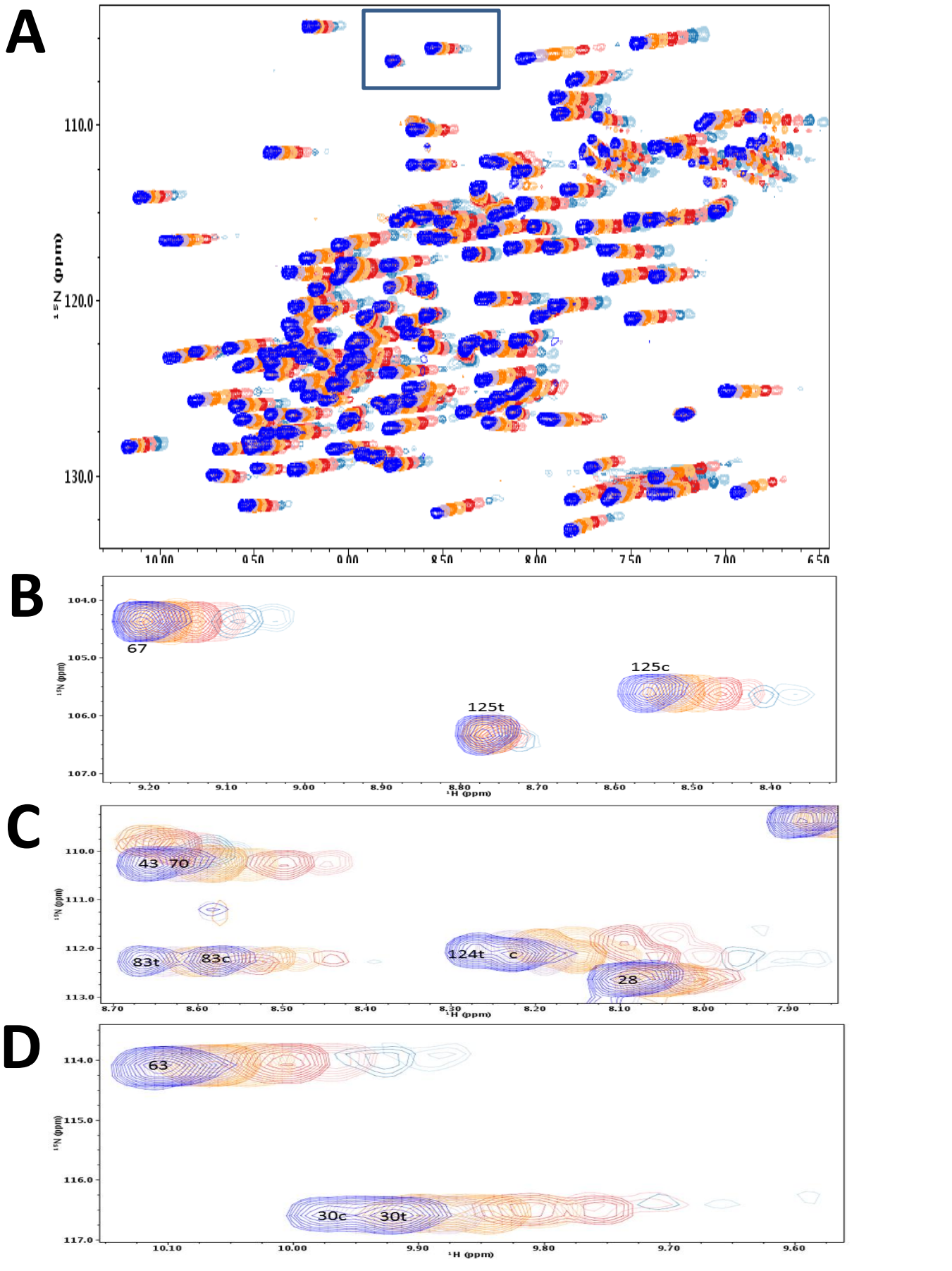
Supplemental Figure S3

Spectra of peptide fingerprinting after annotation. Spectra of peptide finger-printing after annotation were further analyzed by BioTools 3.0 (Bruker Daltonik). The position of the corresponding peptide in the amino acid sequence is given in brackets.



HSQC spectra of wild type Gal-7 and P4L mutant.
^{15}N-^{1}H HSQC Spectrum of wild type Gal-7 (black peaks) is overlaid with an HSQC spectrum of Gal-7 P4L mutant (red peaks). Some doubled resonances in wild type Gal-7 are boxed in, as discussed in the text.

Supplemental Figure S4



Supplemental Figure S5

Temperature dependence of NH resonances. ^{15}N-^{1}H HSQC Spectra are overlaid to illustrate the temperature dependence of NH resonances upon raising the temperature from 278 K to 313 K (**A**). Selected HSQC expansions of these data are shown in panels **B**-**D**. Most resonances in either state are shifted to the same extent, indicating essentially the same potential to form hydrogen bonds. One clear exception is G125 shown in panel **B,** in which the G125 NH in the P4 *trans*-state changes little over this temperature range.