Supplementary Information

Supplementary Methods

MS and MS/MS acquisition and data processing settings

Both LC systems were connected through Thermo Scientific SII for Xcalibur 1.3.0.73 with Chromeleon 7.2.4.8179 for LC control. The acquisition software used was Thermo Foundation 3.1.64.11 with Xcalibur 3.1.66.10 and instrument configuration Q Exactive - Orbitrap MS 2.8 SP1 build 2806.

Comments on acquisition settings and data analysis

The instrument settings commonly used for proteolytic peptides frequently result in failure to acquire MS/MS spectra for larger peptides even though the signal intensity is well above the required threshold. Generally it is desirable to enable the "Peptide match" selection, which would assign the monoisotopic peak *m/z* of the precursor to the fragment io acquisition. This way the precursor *m/z* does not require correction prior to database search. With larger peptides this feature could not be enabled and therefore a more specialized processing program is required, such as Mascot Distiller or PEAKS Studio. Use of these programs are also desirable for other reasons as well. For example, Mascot takes into account only singly and doubly charged fragment ions, and for precursors with higher charge state than 3, fragment ions with charge states >2 are produced. To include these, the software must deconvolute multiply charged ions into singly charged ions (or non-charged species).

We were unable to access a software that did not require prior knowledge of the mass of the link. A program allowing a liberal mass tolerance setting would have been useful; unfortunately a large tolerance of tens or hundreds of Da is typically not allowed. Therefore, the search strategy was to construct a large amount of different PTMs consisting of possible combinations of peptides and links. In the particular case with dimers, PEAKS Studio 8.5 worked well enough since it was possible to perform searches with a large amount of modifications. To speed up the processing we constructed 2 small databases, one containing only APP isoforms and one containing only Aβ1-43.

Once the nature of the link was established, both Mascot Distiller and PEAKS Studio were able to process both intact and tryptic dimer data; PEAKS Studio, however, provided a smoother workflow. We also took advantage of the Xcalibur's built-in Xtract function to charge and isotope deconvolute spectra. The deconvoluted peak lists produced by PEAKS Studio and Xtract differed to some extent and we combined them to obtain more complete fragment ion lists for the intact dimers. The lists were also validated manually against the unprocessed fragment ion acquisition to ensure that the data produced by the algorithms were trustworthy.

Deconvolution algorithms are often very good at computing the correct monoisotopic mass even when the monoisotopic peak is not seen in the spectrum. However, when the signal is not excellent the isotopic envelope is difficult to fit to a theoretical distribution and a mass error of 1 or 2 Da can be the result. This is especially the case with larger fragment ions since signal is lost in the fragmentation process and additional ion transfer. Therefore, the database search software was set to accept an error of 1.2 Da. Further, when analyzing samples such as the Aβ dimers, one should not rely on the database searches for final identification; it is rather a tool to obtain lists of suggestions for putative dimers. Even though it is reassuring to obtain assignments through the database software, it was essential with additional evaluation of the fragment ion spectra. In-house written scripts were used to process deconvoluted fragment ion data both from PEAKS Studio and Xcalibur's Xtract function and obtain lists of matching b- and y-series, which assisted in the identification.

The scores given by PEAKS Studio were low for the dimers (the scores for the monomer data is in a different league). The search engine is, however, not adapted to dimeric species (one of the chains was treated as a PTM) and the given scores are difficult to interpret. We chose to include them anyway, but have also supplied the number of manually validated b-and y-ions. Supplementary Table 2 shows all acquisitions from one LC-MS/MS run where the fragment ion data clearly supported the molecular species. In the table the mass deviation for the precursor masses are given both in ppm and Da; it can be seen that the deviation is very close to an integer value, which fits well with an isotope mismatch of up to 2 Da. Moreover, in the precursor mass spectra (Fig. 3b and Supplementary Fig. 13) it can be seen that there was an extensive overlap of species with similar *m/z* and retention time making accurate assignment of the monoisotopic peak very difficult. Since there was an abundance of ions detected in the precursor acquisitions, the injection times also became relatively short; hence the true ion signal was low for every molecular ion, contributing to the noisy appearance. Indeed, we set the acquisition range to 1200-2000 *m/z* units in order to obtain good data for the dimers; a normal acquisition range of 400-2000 *m/z* units produced essentially no signal above *m/z* 1200.

The situation was very different for the MS/MS acquisitions, which due to the narrow isolation window of 3 *m/z* units could have long injection times and therefore a comparatively good signal could be obtained for the fragment ions belonging to the isolated species. Here the spectra were quite clean with low background, allowing for decent deconvolution conditions as well as good manual inspection conditions. The problem with incorrect monoisotopic assignment was still there, but for these peaks (in our case rarely suffering from overlap) the error was almost always either ~0 Da or ~+1 Da. Because of the shape of the isotopic distribution an isotope mismatch error will always have a positive value unless there are peak overlaps. In the end all MS and MS/MS acquisitions presented were carefully examined manually and fragment ion acquisitions not having a clear Aβ fragment profile, as well as a fitting precursor ion mass, were discarded. All approved MS/MS acquisitions had fragment intensity distributions matching those of monomeric Aβ, particularly the characteristic high abundance b-ions in the b30-b40 range which can be seen in Supplementary Figs. 11-13.

Spectra from digested samples were also subjected to analysis by Trans-Proteomic Pipeline/Kojak. This software allows analysis of linked peptides. Also, here the link mass has to be known beforehand, which limits the usefulness when the objective is to screen for peptides with and endogenous, unknown link. Nevertheless, once the number of linking possibilities had been narrowed down to water and ammonia loss TPP/Kojak was a handy tool to confirm findings and also suggest other linked peptide variants.

Hitherto, we have not found a really smooth workflow but are still relying on a combination of software with some manual data handling in between. By using in-house developed scripts simpler data extraction can be semi-automated, which reduces analysis time significantly.

Mascot Daemon search parameters – search using Mascot Distiller for spectrum processing

All searches [Database = custom made Abeta1-43, APP human isoforms, Uniprot_SwissProt; Fixed modifications = none; Variable modifications = Oxidation (M), Glu–>pyro-Glu (N-term E), and various “dimer PTMs”; Decoy = not enabled; Enzyme = none; Max. missed cleavages = not relevant; Monoisotopic = selected; Peptide charge = 1+; Peptide tol. = 20 ppm (digested samples)/1.2 Da (intact samples); #13C = 0].

MS/MS [MS/MS ion search = enabled; Error tolerant search = not enabled; Data format = Mascot generic; MS/MS tolerance = 50 mmu (digested samples)/1.2 Da (intact samples); Quantitation = none; instrument type = CID fragment type spectra – all singly charged *b*- and *y*-ions].

Data import filter = Mascot Distiller [Data File Format = ThermoXcalibur; Default for unknown scan type = Profile/continuum; Data import filter options: Mascot Distiller Processing Options = see below; Multi-Sample Files = Separate search for each sample; Peak List Format = MGF; Intensity values = Area; Scan Range (multi-scan files) = sample dependent; Distiller Project File Save = enabled; Output PMF Masses as = MH+; Output MS/MS Fragments as = MH+].

Mascot Distiller Processing Options

MS Processing: Un-centroiding [Peak half width = 0.025; Data points per Da = 100; Data points per Da = 100; Always uncentroid = enabled]; Re-gridding [Data points per Da = 100]; Multi-Format Spectrum [Preferred type = Profile]; Peaks [Minimum number = 1; Maximum charge = 15]; Aggregation [Scan group aggregation method = Sum].

MS/MS Processing: Un-centroiding [Peak half width = 0.025; Data points per Da = 100; Data points per Da = 100; Always uncentroid = enabled]; Re-gridding [Data points per Da = 100]; Multi-Format Spectrum [Preferred type = Profile]; Peaks [Minimum number = 8; Maximum charge = N/A; Use precursor charge as maximum = enabled]; Precursor Charge [1st choice = Try to re-determine charge from parent scan; 2nd choice = If available, take charge from file; 3rd choice = Use default charge(s); Default charge range = 2 to 15; Ignore singly charged precursors = not enabled]; Precursor Selection [Search within m/z tolerance of = 2.5 Da; Re-determine precursor m/z value when possible = enabled; Maximum number of precursor m/z values = 1]; Aggregation [Scan group aggregation method = Time Domain].

Time Domain: Group assignment [Minimum precursor mass (Mr) = 700; Maximum precursor mass (Mr) = 16 000; Precursor m/z tolerance = 0.01; Maximum intermediate time (secs) = 0; Maximum intermediate scan count = dimmed; Use intermediate scan count when possible = not enabled]; Group Filtering [Minimum number of scans = 1]. Group combination [Sum MSn scans into MS2 = enabled].

MS Peak Picking: Filtering [Correlation threshold (Rho) = 0.5; Minimum signal to noise (S/N) = 5; Minimum peak m/z = 50; Maximum peak m/z = 100 000]; Peak profile [Minimum peak width

(Da) = 0.001; Expected peak width (Da) = 0.025; Maximum peak width (Da) = 0.5; Reject width outliers = not enabled]; General [Apply baseline correction = not enabled; Fit method = Isotope Distribution; Maximum peak iterations per scan = 500]; Single Peak Window [Pick single peaks in this range (e.g. reporter ions) = not enabled; other parameters dimmed].

MS/MS Peak Picking: General [Same as MS Peak Picking = enabled; other parameters dimmed].

PEAKS Studio 8.5 processing parameters (typical)

Create Project options: [Instrument type = Orbitrap (Orbi-Orbi); Fragment = HCD]. Data Refinement options: [Merge Scans = not enabled (except for intact #1185 dimer sample); Correct Precursor = enabled; Mass only (recommended) = enabled; Filter Scans = not enabled]. Identification options: [Error Tolerance: Precursor mass = 20 ppm (digested samples)/1.2 Da (intact samples) using monoisotopic mass; Fragment ions = 0.05 Da (digested samples)/1.2 Da (intact samples); Enzyme = None; Selected Fixed PTM = none; Selected Variable PTM = Oxidation (M), Pyro-glu from E, and various “dimer PTMs”; max variable PTM per peptide = 3 to 6; Database = custom made Abeta1-43, APP human isoforms; Uniprot_SwissProt].

Specific PEAKS Studio 8.5 processing parameters for scores given in Supplementary Table 1

Create Project options: [Instrument type = Orbitrap (Orbi-Orbi); Fragment = HCD]. Data Refinement options: [Merge Scans = not enabled; Correct Precursor = enabled; Mass only (recommended) = enabled; Filter Scans = not enabled]. Identification options: [Error Tolerance:

Precursor mass = 20 ppm using monoisotopic mass; Fragment ions = 0.05 Da; Enzyme = None; Selected Fixed PTM = none; Selected Variable PTM = Oxidation (M), Pyro-glu from E, Deamidation (NQ), Formylation(K, peptide N-term); Hydrogen dodecyl sulfate adduct; max variable PTM per peptide = 3; Database = custom made Abeta1-43].

Specific PEAKS Studio 8.5 processing parameters for scores given in Supplementary Table 2

Create Project options: [Instrument type = Orbitrap (Orbi-Orbi); Fragment = HCD]. Data Refinement options: [Merge Scans = not enabled; Correct Precursor = enabled; Mass only (recommended) = enabled; Filter Scans = not enabled]. Identification options: [Error Tolerance: Precursor mass = 1.2 Da using monoisotopic mass; Fragment ions = 1.2 Da; Enzyme = None; Selected Fixed PTM = none; Selected Variable PTM = Oxidation (M), Pyro-glu from E, Formylation (K, peptide N-term); Hydrogen dodecyl sulfate adduct, and 25 “dimer PTMs” with -H_2O link (Ab1-37, 1-38, 1-39, 1-40, 1-42, 2-37, 2-38, 2-39, 2-40, 2-42, 3-37, 3-38, 3-39, 3-40, 3-42, Pyro-glu3-37, Pyro-glu3-38, Pyro-glu3-39, Pyro-glu3-40, Pyro-glu3-42); max variable PTM per peptide = 3; Database = custom made Abeta1-43].

Trans-Proteomic Pipeline/Kojak processing parameters

Contents of the Kojak .conf parameter file:

```
# Kojak version 1.5.5 parameter file

# Please see online documentation at:

# http://www.kojak-ms.org/param

# All parameters are separated from their values by an equals sign ('=')

# Anything after a '#' will be ignored for the remainder of the line.

#

# Computational resources

threads    =   4  #Increase to use more cores/nodes

#

# Data input files: include full path if not in current working directory

#

database        =        c:/TPP/data/dbase/Abeta.fasta        # local Abeta database

export_percolator      =        1

export_pepXML        =        1

MS_data_file  =        my_data.mzML

percolator_version     =        3.0

#

# Parameters used to described the data being input to Kojak

#

enrichment     =        0        #Values between 0 and 1 to describe 18O APE.

                                 #For example, 0.25 equals 25 APE.

instrument     =        0        #Values are: 0=Orbitrap, 1=FTICR (such as Thermo LTQ-FT)
```

MS1_centroid = 0 #0=no, 1=yes

MS2_centroid = 1 #0=no, 1=yes

MS1_resolution = 50000 #Resolution at 400 m/z, value ignored if data are

#already centroided

MS2_resolution = 50000 #Resolution at 400 m/z, value ignored if data are

#already centroided

#

Cross-link and mono-link masses allowed. May have more than one of each parameter.

#

Format for cross_link is [amino acids] [amino acids] [mass mod] [identifier]

Format for mono_link is [amino acids] [mass mod]

One or more amino acids (uppercase only!!) can be specified for each linkage moiety

Use lowercase 'n' or 'c' to indicate protein N-terminus or C-terminus

#

cross_link = ACDEFGHIKLMNPQRSTVWY ACDEFGHIKLMNPQRSTVWY -18.010565

-H2O

#

Fixed modifications. Add as many as necessary.

#

fixed_modification = C 57.02146

fixed_modification_protC = 0

fixed_modification_protN = 0

```
#
# Differential modifications. Add as many as necessary. Uppercase only for amino acids!
# n = peptide N-terminus, c = peptide C-terminus
#
# If more than one modification is possible for an amino acid,
# list all modifications on separate lines
#
modification	=	M	15.9949
modification_protC	=	0
modification_protN	=	0
diff_mods_on_xl	=	0
max_mods_per_peptide	=	2
mono_links_on_xl	=	0
#
# Digestion enzyme rules.
#
# See http://www.kojak-ms.org/param/enzyme.html
#
enzyme	=	[DKR]|{P} All_Abeta	# when entering all amino acids searches failed
#
# Scoring algorithm parameters
#
```

```
# fragment_bin_offset and fragment_bin_size influence algorithm precision and memory usage.
# They should be set appropriately for the data analyzed.
# For ion trap ms/ms:  1.0005 size, 0.4 offset
# For high res ms/ms:    0.03 size, 0.0 offset
#
fragment_bin_offset  =       0.4       #between 0.0 and 1.0
fragment_bin_size    =       1.0005 #in Thomsons
ion_series_A   =       0
ion_series_B   =       1
ion_series_C   =       0
ion_series_X   =       0
ion_series_Y   =       1
ion_series_Z   =       0        #Z-dot values are used
#
# Additional parameters used in Kojak analysis
#
decoy_filter    =      DECOY #identifier for all decoys in the database.
                             #Default value is "random" (without quotes)
isotope_error  =       1        #account for errors in precursor peak identification.
                                #Searches this number of isotope peak offsets.
                                #Values are 0,1,or 2.
max_miscleavages     =     2       #number of missed trypsin cleavages allowed
```

```
max_peptide_mass    =    5000.0 #largest allowed peptide mass in Daltons
min_peptide_mass    =    400.0  #lowest allowed peptide mass in Daltons
max_spectrum_peaks  =    0      #top N peaks to use during analysis. 0 uses all peaks.
ppm_tolerance_pre   =    15.0   #mass tolerance on precursor when searching
prefer_precursor_pred    =      2    #prefer precursor mono mass predicted by
                                     #instrument software.
                                # 0 = ignore previous predictions
                                # 1 = use only previous predictions
                                # 2 = supplement predictions with additional analysis
spectrum_processing =    0      #0=no, 1=yes
top_count     =    300   #number of top scoring single peptides to combine
                         #in relaxed analysis
truncate_prot_names =    0      #Max protein name character to export, 0=off
turbo_button        =    1      #Generally speeds up analysis. Special cases cause reverse
                                #effect, thus this is allowed to be disabled. 0=off
```

Xtract processing parameters (typical)

Resolution@400 = 50 000; S/N Threshold = 2; Fit Factor = 75%; Remainder = 25%; Averagine Table = Averagine; Max Charge = 6. Generate Masses Mode = $[M+H]^+$.

Algorithm for combining deconvoluted peak lists from PEAKS Studio and Xtract

While PEAKS Studio was superior to Xtract to deconvolute peaks in the lower *m/z* segment Xtract was slightly better in for larger ions. Apart from that neither program produced a peak list incorporating all peaks produced by the other program, the calculated peak areas were different. The areas were not used for quantification but the actual numbers differed enough making it impossible to show them in the same graph, so a simple harmonization was required. This was done by choosing one common low mass and one common high mass peak from the output of the respective programs, calculating the Xtract-to-PEAKS Studio area ratios, calculating intercept and slope for a line containing the two ratios, and applying this mass dependent normalization factor to the PEAKS Studio area numbers. The two peak lists were then combined.

Supplementary Figure Legends

Supplementary Fig. 1 Treatment of iNs with aqueous AD brain extracts induces neuritic dystrophy. (**a**) Schematic depicts the process used to generate mature iNs and the time interval for sample addition and live cell imaging. (**b**) On iN day 21, cells were treated with medium alone (control) or brain extracts (#1242-mock and #1242-ID) and cells imaged for 72 hours. Phase contrast images (top panel) were used to identify neurites (middle panel) using IncuCyte NeuroTrack software. Identified neurites (purple) are shown on the phase contrast images (bottom panel). Scare bars are 100 µm. (**c**) Time-course plots show that Aβ-containing aCSF extracts of brains #1242 (red filled circle) and #722 (blue filled circle) cause neuritotoxicity compared to the medium alone control (black) (comparison over last 6 hours of recording: #1242-mock vs. control, $p<0.001$; #722-mock vs. control, $p<0.001$; one-way ANOVA), or brain extracts immunodepleted (ID) of Aβ with AW7; #1242-ID (red open circle) and #722-ID (blue open circle) (comparison over last 6 hours of recording:#1242-mock vs. ID, $p<0.001$; #722-mock vs. ID, $p<0.001$; one-way ANOVA). Each well of iNs was imaged for 6 h prior to addition of sample and NeuroTrack-identified neurite branch points used to normalize neurite branch points measured at each interval after addition of sample. Cells treated with medium alone were used to monitor the integrity of untreated cells.

Supplementary Fig. 2 Aqueous extract of mild AD brain contain ~4 and ~7 kDa Aβ species, which are immunologically indistinguishable from those from end-stage AD brain. (**a**) aCSF extract of mild AD brain #1670 was IP'd with AW7-beads, antigen eluted with 500 mM ammonium hydroxide, the eluate lyophilized, the lyophilizate dissolved in formic acid and the resulting solution subjected to SEC, and fractions used for WB with 2G3+21F12. (**b**) SEC-isolated ~4 and ~7 kDa fractions from mild AD brain #1670 and end-stage AD brain #722 were used for WB'ing employing 6 different anti-Aβ mAbs. Synthetic Aβ1-40, Aβ1-42 and recombinant NTE-Aβ (-31Aβ1-42) and Aη-α peptides were loaded as controls. Single arrow and double arrows indicate the ~4 and ~7 kDa Aβ species, respectively, and an asterisk marks the position of Aη-α. The ~7 kDa Aβ species from mild AD brain #1670 and end-stage AD brain #722 co-migrate and exhibit similar immunoreactivity anti-Aβ mAbs.

Supplementary Fig. 3 The ~7 kDa Aβ species are not induced during the purification processes. (**a**) aCSF-B buffer without (upper panel) or with (lower panel) 100 ng/mL synthetic Aβ1-42 was IP'd with AW7-beads, antigen eluted with 500 mM ammonium hydroxide, the eluate lyophilized, the lyophilizate dissolved in formic acid and the resulting solution subjected to SEC, and fractions used for WB with 4G8. (**b**) aCSF-B extract of control brain #1821 without (upper panel) or with (lower panel) 100 ng/mL synthetic Aβ1-42 was IP'd with AW7-beads, antigen eluted with 500 mM ammonium hydroxide, the eluate lyophilized, the lyophilizate dissolved in formic acid and the resulting solution subjected to SEC, and fractions used for WB with 4G8. No signal was detected in fractions 8-10, where the ~7 kDa Aβ species elute.

Supplementary Fig. 4 Both aqueous ~7 kDa Aβ and plaque-derived ~7 kDa Aβ are neuritotoxic. The effect of ~7 kDa Aβ from brain #1242 on neuritic branch points was quantified using the same neurons shown in Figure 1**e** and Figure 2**e**. (**a**) Time-course lots show that the aqueous ~7 kDa Aβ, but not Aβ monomer, caused time-dependent neuritotoxicity (comparison over last 6 hours of recording: ~7 kDa Aβ vs. control, $p<0.01$; ~4 kDa Aβ vs. control, $p>0.05$; one-way ANOVA). (**b**) Branch points of the Aβ monomer and ~7 kDa Aβ treated iNs as shown in Figure 2**e**. Time-course lots show that the ~7 kDa Aβ from AD amyloid plaques, but not Aβ monomer, caused time-dependent neuritotoxicity (comparison over last 6 hours of recording: ~7 kDa Aβ vs. control, $p<0.001$; ~4 kDa Aβ vs. control, $p>0.05$; one-way ANOVA).

Supplementary Fig. 5 AW7 immunodepletion removes neuritotoxicity induced by the ~7 kDa Aβ fractions. (**a**) aCSF extract of AD brain #414 was IP'd with AW7-beads, antigen eluted with 500 mM ammonium hydroxide, the eluate lyophilized, the lyophilizate dissolved in formic acid and the resulting solution subjected to SEC, and fractions used for WB with 4G8. (**b**) The Aβ monomer and ~7 kDa Aβ fractions shown in **a** were exchanged into iN culture medium, immunodepleted with pre-immune serum or AW7, and then added to iN cells. The ~7 kDa Aβ, but not Aβ monomer, caused time-dependent neuritotoxicity. AW7 immunodepletion removes the neuritotoxicity of the ~7 kDa Aβ.

Supplementary Fig. 6 LC-MS identifies a rich array of monomer primary structures in aqueous brain extract. (**a**) aCSF extract of brain #1185 was IP'd with AW7-beads and used for SEC as described in the Methods, and fractions analyzed by WB with 2G3 and 21F12. The fractions which contained ~7 kDa Aβ and monomers were used for the mass spectrometric analysis shown in Fig. 1**f** and **g**. (**b**) Spectra are shown for 4 chromatograph retention time spans for the SEC-isolated monomer fraction of brain #1185 aCSF extract. The x-axis indicates *m/z* values between 850 and 1350, the y-axis signal intensity, and the z-axis the HPLC retention time span. The identities of the peaks shown were confirmed by MS/MS.

Supplementary Fig. 7 Plaque-derived ~7 kDa Aβ species from AD brain #722 is neuritotoxic. . (**a**) Amyloid plaques isolated from AD brains #722 were dissolved in formic acid, chromatographed on SEC and analyzed by WB with 2G3 and 21F12. (**b** and **c**) Equal amount of the Aβ monomer and ~7 kDa Aβ fractions shown in **a** were applied to iNs. Time-course plots of relative neurite length (**b**) and branch points (**c**) show that plaque-derived ~7 kDa Aβ species (red) cause neuritotoxicity, whereas plaque-derived Aβ monomer (blue) does not (comparison over last 6 hours of recording: ~7 kDa Aβ vs. control, $p<0.001$; ~4 kDa Aβ vs. control, $p>0.05$; one-way ANOVA). The medium vehicle control is shown in black.

Supplementary Fig. 8 The ~7 kDa Aβ species isolated from plaques co-migrate with the ~7 kDa Aβ in aCSF brain extracts. (**a**) A total of 8 mAbs were used to investigate the primary structure of plaque-derived and aCSF extracted Aβ. (**b**) Plaque SEC-isolated ~4 and ~7 kDa fractions, and AW7 IPs of aCSF extracts were used for WB'ing employing 6 different anti-Aβ mAbs, and (**c**) 2 mAbs with epitopes in APP N-terminal of Aβ. The ~7 kDa Aβ species from aCSF extracts and solubilized plaques co-migrate and react similarly with anti-Aβ mAbs, but are not recognized by the anti-APP mAbs 2E9 or 28D10. (**c**) Re-probing the 28D10 blot with 4G8 reveals ~4 and ~7 kDa Aβ species are present. Synthetic Aβ1-40, Aβ1-42, recombinant NTE-Aβ (-31Aβ1-42) and recombinant Aη-α were loaded as controls. A single arrow indicates Aβ monomer, double arrows ~7 kDa Aβ, and an asterisk denotes Aη-α.

Supplementary Fig. 9 Western blot analysis of plaques isolated from brain #1444. Amyloid plaques from AD brain #1444 were dissolved in formic acid, chromatographed on SEC and analyzed by WB with 2G3 and 21F12. The elution of Blue dextran (BD) and globular protein standards is indicated by downward point arrows and SDS-PAGE molecular weight standards are on the left. Single arrow and double arrows indicate the ~4 and ~7 kDa Aβ, respectively. Synthetic Aβ1-42 loading controls are in the last 3 lanes. Fractions (8-10) containing ~4 kDa and fractions (13-15) containing ~7 kDa Aβ were pooled and used for LTP experiments shown in Fig. 2**f** and **g**.

Supplementary Fig. 10 LC-MS identifies a rich array of plaque-derived monomer primary structures both within and between brains. Spectra are shown for 4 chromatograph retention time spans for plaque-derived SEC-isolated monomer fractions of brains #1185, #1444, #722, #1167, #1242, and #464. The x-axis indicates *m/z* values between 850 and 1350, the y-axis signal intensity, and the z-axis the HPLC retention time span. The identities of the peaks shown were confirmed by MS/MS (see Supplementary Table 1). Approximately 10% of the respective SEC-isolated fractions was used for LC-MS and -MS/MS analysis.

Supplementary Fig. 11 Deconvoluted fragment ion spectrum of the plaque-derived intact dimer Aβ1-40×1-40 from brain 1242. The schematic shows an Aβ1-40 homo-dimer cross-linked between D1 and E22. The α-chain is shown in green and the β-chain in orange, and fragmentation sites corresponding to detected fragments are indicated. Deconvoluted peak centroids for plaque-derived intact ~7 kDa Aβ from brain #1242 are shown in 3 separate panels, $[M+H]^+$: 0-2,500 (upper panel), 2,500-6,500 (middle panel), and 6,500-8,700 (lower panel). Peak centroids are below the labels with a help line above as guide for the amino acid ladders indicated. Peaks from three different fragment ion series are indicated together with the respective sequence ladders; α-chain b-ions (green), β-chain y-ions (italic orange), and α(1-40)×β(1-40)-chain b-ions (blue). Unassigned peaks are in light grey. Only one ladder is observed, indicating that for an individual dimer ion only one of the chains is subject to fragmentation (cf. Supplementary Fig. 14). However, peaks corresponding to cleavages between E22 and D1 must originate from the β-chain. Approximately 10% of the SEC-isolated fraction was used for this LC-MS/MS analysis. Supplementary Table 3 contains the data presented in this figure.

Supplementary Fig. 12 Deconvoluted fragment ion spectrum of the intact Aβ1-40×1-38 and Aβ1-38×1-40 heterodimer from brain 1242. The schematic shows two possible Aβ1-40xAβ1-38 hetero-dimers cross-linked between D1 and E22. The α-chain is shown in green for 1-40 on the left panel, and 1-38 or the right panel. The β-chain is in blue for 1-38 on the right panel, and in orange for 1-40 of the left panel. Fragmentation sites corresponding to detected fragments are indicated. Deconvoluted peak centroids for plaque-derived intact ~7 kDa Aβ from brain #1242 is shown in 3 panels with $[M+H]^+$ ranging from: 0-2,500 (upper panel), 2,500-6,500 (middle panel), and 6,500-8,500 (lower panel). Peak centroids are below the labels with a help line above as guide for the amino acid ladders indicated. Peaks from five different fragment ion series are indicated with the respective sequence ladders; α-chain b-ions (green), β(1-38)-chain y-ions (italic blue), β(1-40)-chain y-ions (italic orange), α(1-40)×β(1-38)-chain b-ions (blue), and α(1-38)×β(1-40)-chain b-ions (orange). Unassigned peaks are in light grey. Two ladders are observed (one for each dimer type) indicating that only one chain (presumably the β-chain) from each dimer type is subject to fragmentation. Approximately 10% of the SEC-isolated fraction was used for this LC-MS/MS analysis. Supplementary Table 3 contains the data presented in this figure.

Supplementary Fig. 13 Deconvoluted fragment ion spectrum of the plaque-derived intact dimer Aβ1-42×1-42 from brain #1185. The upper left panel shows the ion chromatogram for *m/z* 1502.76. The average mass spectrum of the indicated retention time window and the fragment mass spectrum was generated by averaging all MS/MS acquisitions for *m/z* 1502.76 within the time window. Expansions around *m/z* 1502.76 are shown together with the theoretical isotope distributions for Aβ1-42 homo-dimer 6+ ions having links with either NH_3 or H_2O net loss. The schematic at the upper right shows an Aβ1-42 homo-dimer. The α-chain is shown in green and the β-chain in orange, and all fragmentation sites corresponding to detected fragments are indicated. The deconvoluted peak centroids of the fragment mass spectrum for plaque-derived intact ~7 kDa Aβ from brain #1185 are shown in 3 separate panels, $[M+H]^+$: 0-2,500 (upper panel), 2,500-6,500 (middle panel), and 6,500-9,100 (lower panel). Peak centroids are below the labels with a help line above as guide for the amino acid ladders indicated. Peaks from three different fragment ion series are indicated together with the respective sequence ladders; α-chain b-ions (green), β-chain y-ions (italic orange), and α(1-

42)×β(1-42)-chain b-ions (blue). Unassigned peaks are shown in light grey. Only one ladder is observed, indicating that for an individual dimer ion only one of the chains is subject to fragmentation (cf. Supplementary Fig. 14). Approximately 50% of the SEC-isolated fraction was used for this LC-MS/MS analysis. Supplementary Table 3 contains the data presented in this figure, with mass deviations for both types of links (NH_3 or H_2O net loss).

Supplementary Fig. 14 Deconvoluted fragment ion spectrum of dityrosine dimer. Dimers were formed by enzymatic oxidation of recombinant Aβ(1-42) to generate 1-42 homodimers linked between Y10 of one monomer chain and the Y10 of the opposing monomer and an expected monoisotopic $[M+H]^+$ of 9,021.53 Da. The deconvoluted peak centroids of the spectrum spanning the $[M+H]^+$ from 7,100 to 9,100 are shown. Fragment ions corresponding to simultaneous fragmentation of both the α- and β-chains is evident, but since the α- and β-chains are equivalent, annotations only refer to dimers for which the α-chains are longer. Fifteen pmol Y10-linked Aβ1-42×1-42 was used for this LC-MS/MS analysis. Supplementary Table 3 contains the data presented in this figure.

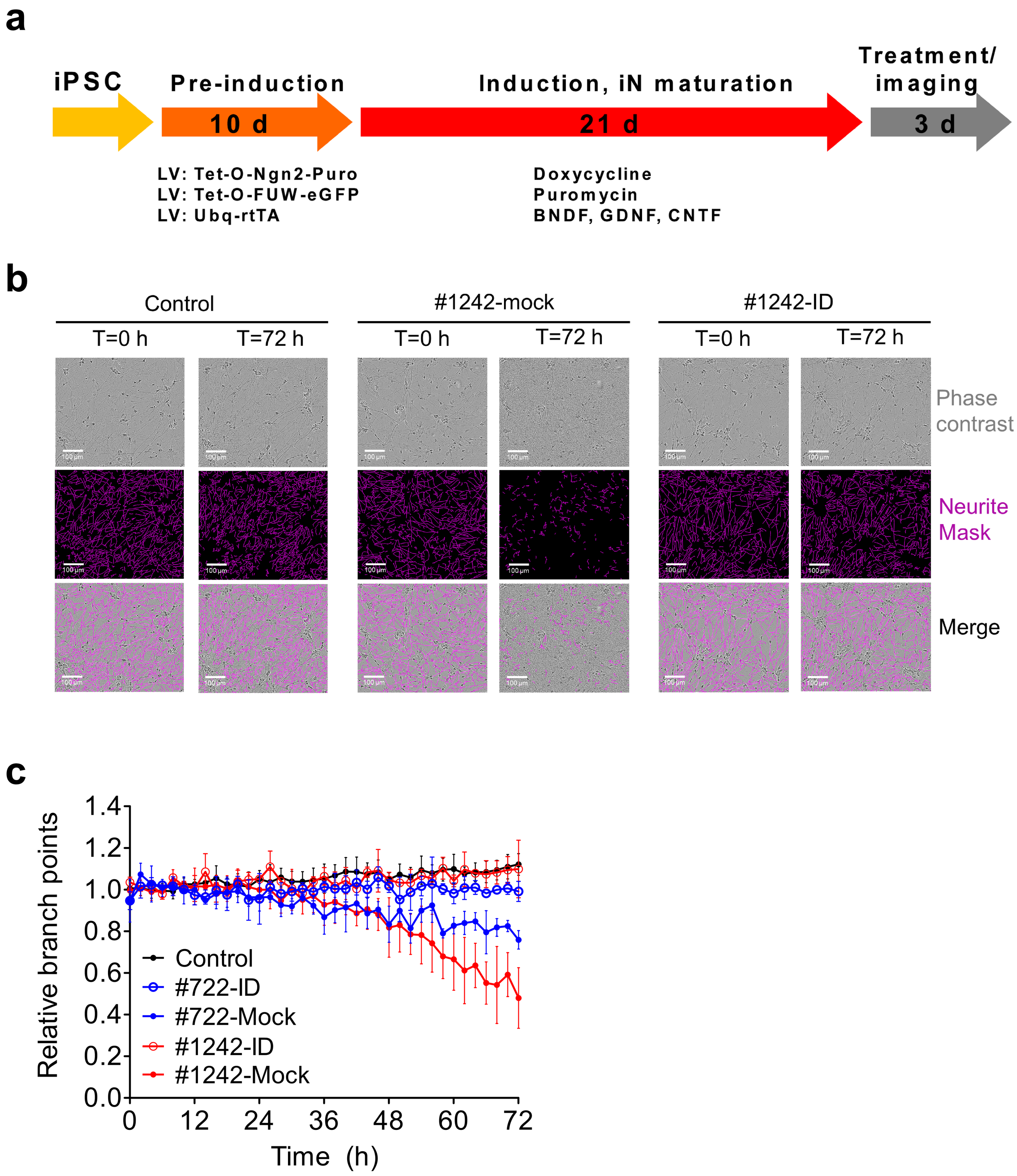
Supplementary Fig. 15 Detailed fragment ion spectrum of the tryptic peptide Aβ17-28×1-5 from the ~7 kDa plaque-derived fraction of brain #1242. (**a**) Deconvoluted fragment ion spectrum from tandem MS/MS of the tryptic peptide Aβ17-28x1-5 with all identified peaks indicated both with sequence and using the nomenclature based on Ref. (Schilling *et al.*, 2003) extended with internal fragments. Peaks corresponding to identified Aβ sequence are colored and unassigned peaks are in light grey. (**b**) Schematic of the tryptic peptides released from a putative Aβ1-40-Aβ1-40 dimer cross-linked at D1 and E22, and Aβ17-28×1-5 related fragments detected in the ~7 kDa plaque-derived fraction isolated from brain #1242. Aβ heterodimers are covalently cross-linked and the most abundant species is linked at E22 and D1. Supplementary Table 4 contains the data presented in this figure.

Supplementary Fig. 16 Full length version of the blots shown in Fig. 1 and 2.

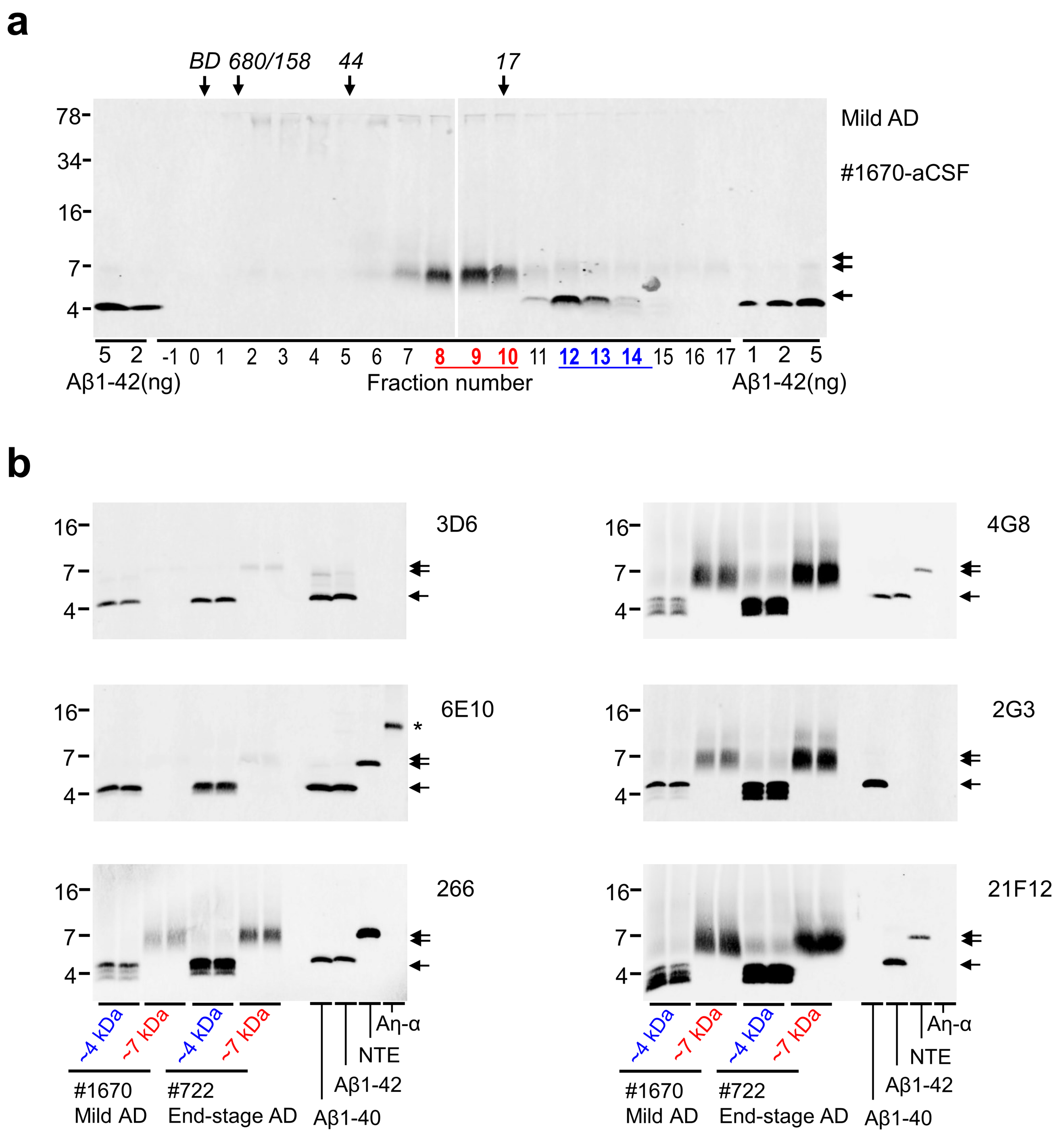
References

Schilling B, Row RH, Gibson BW, Guo X, Young MM. MS2Assign, automated assignment and nomenclature of tandem mass spectra of chemically crosslinked peptides. Journal of the American Society for Mass Spectrometry 2003; 14(8): 834-50.

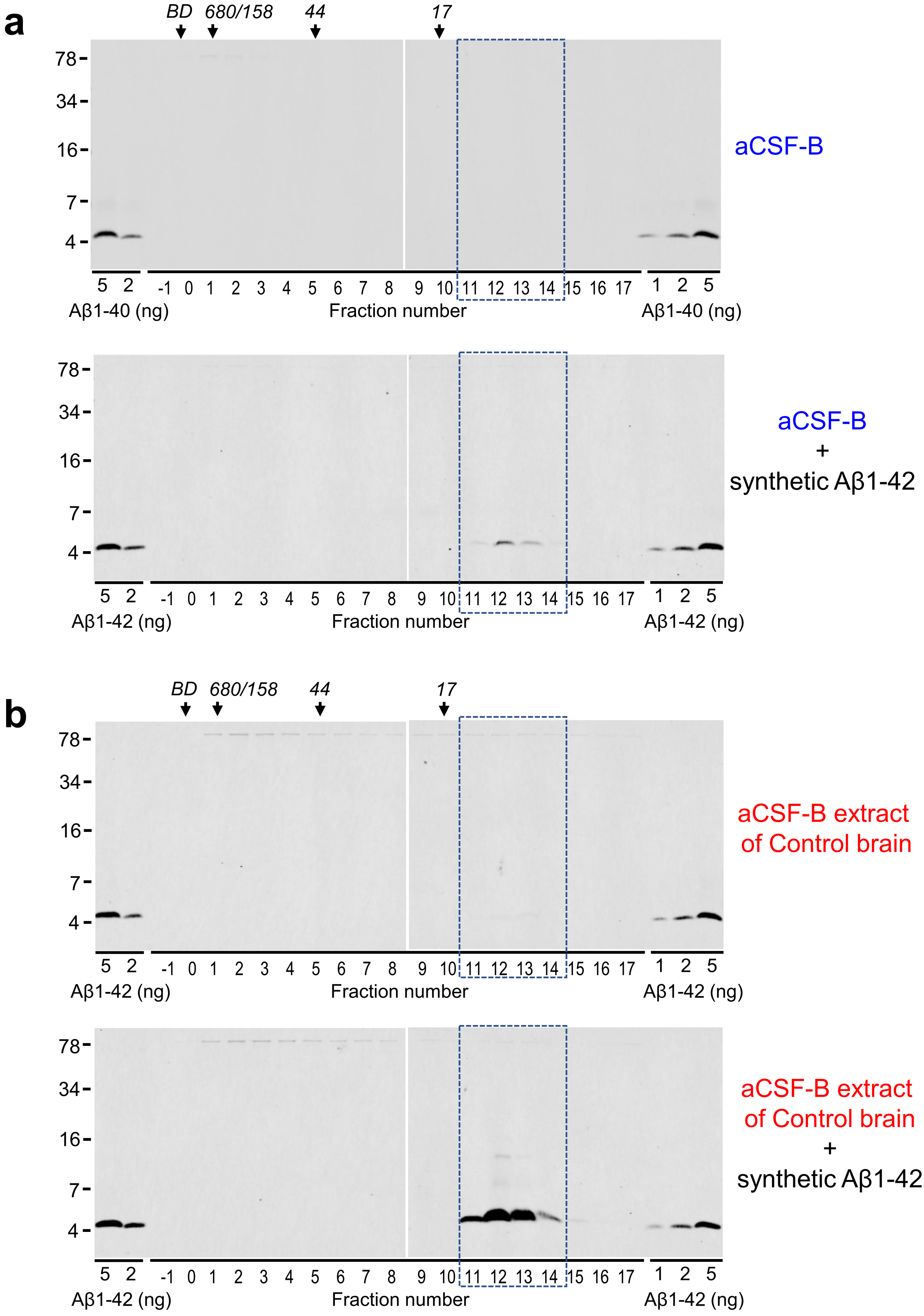
Supplementary Fig. 1



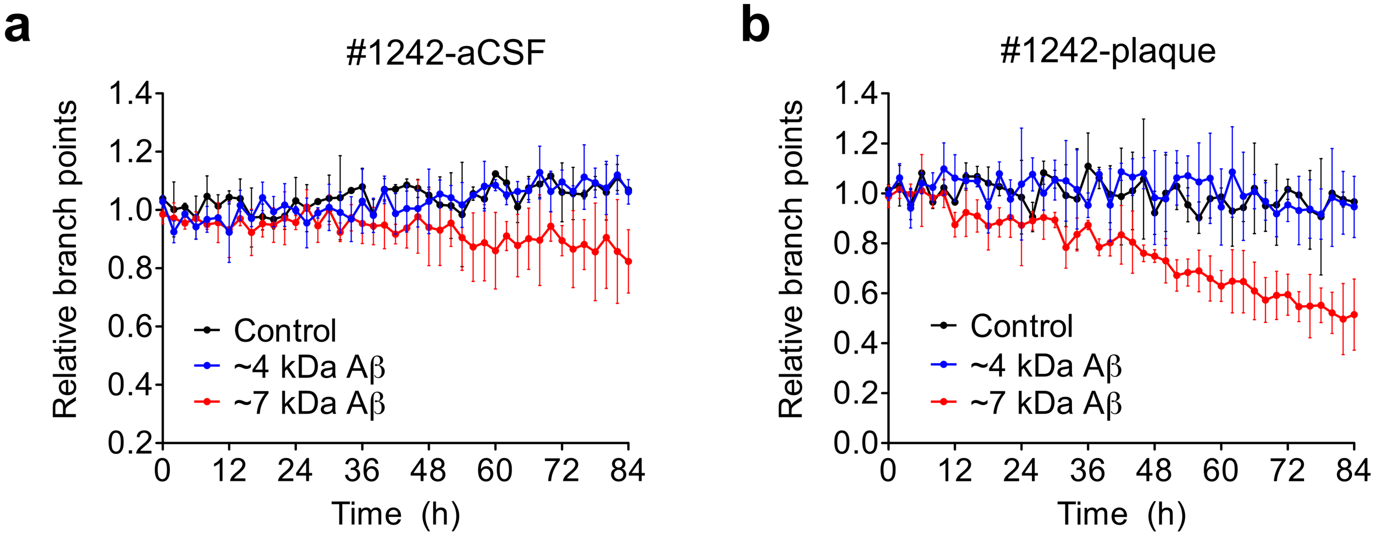
Supplementary Fig. 2



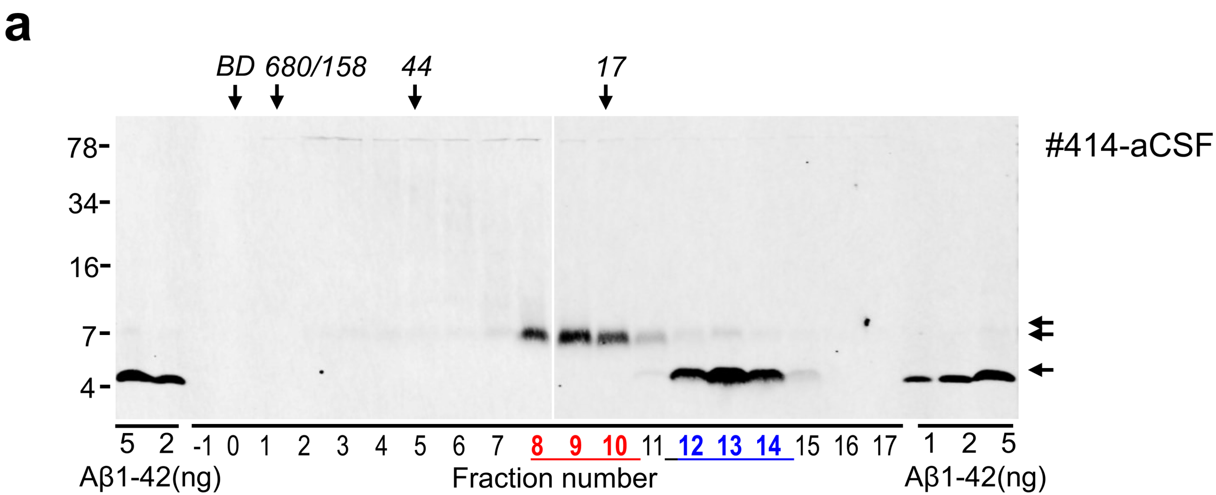
Supplementary Fig. 3

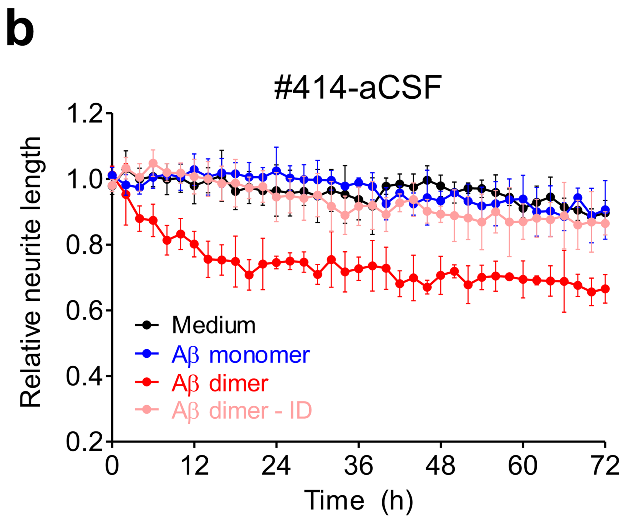


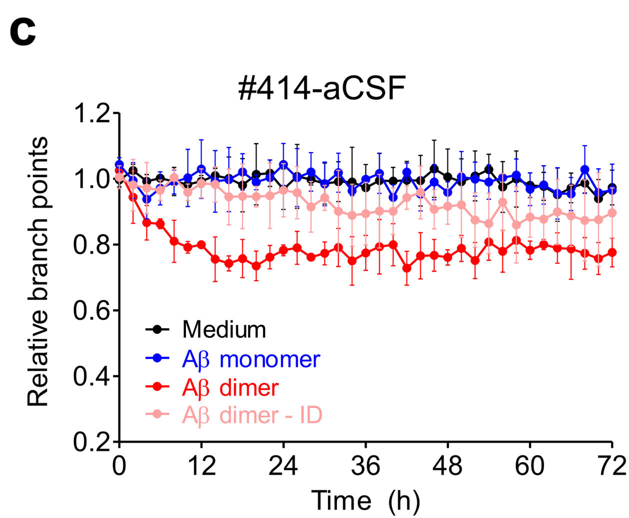
Supplementary Fig. 4



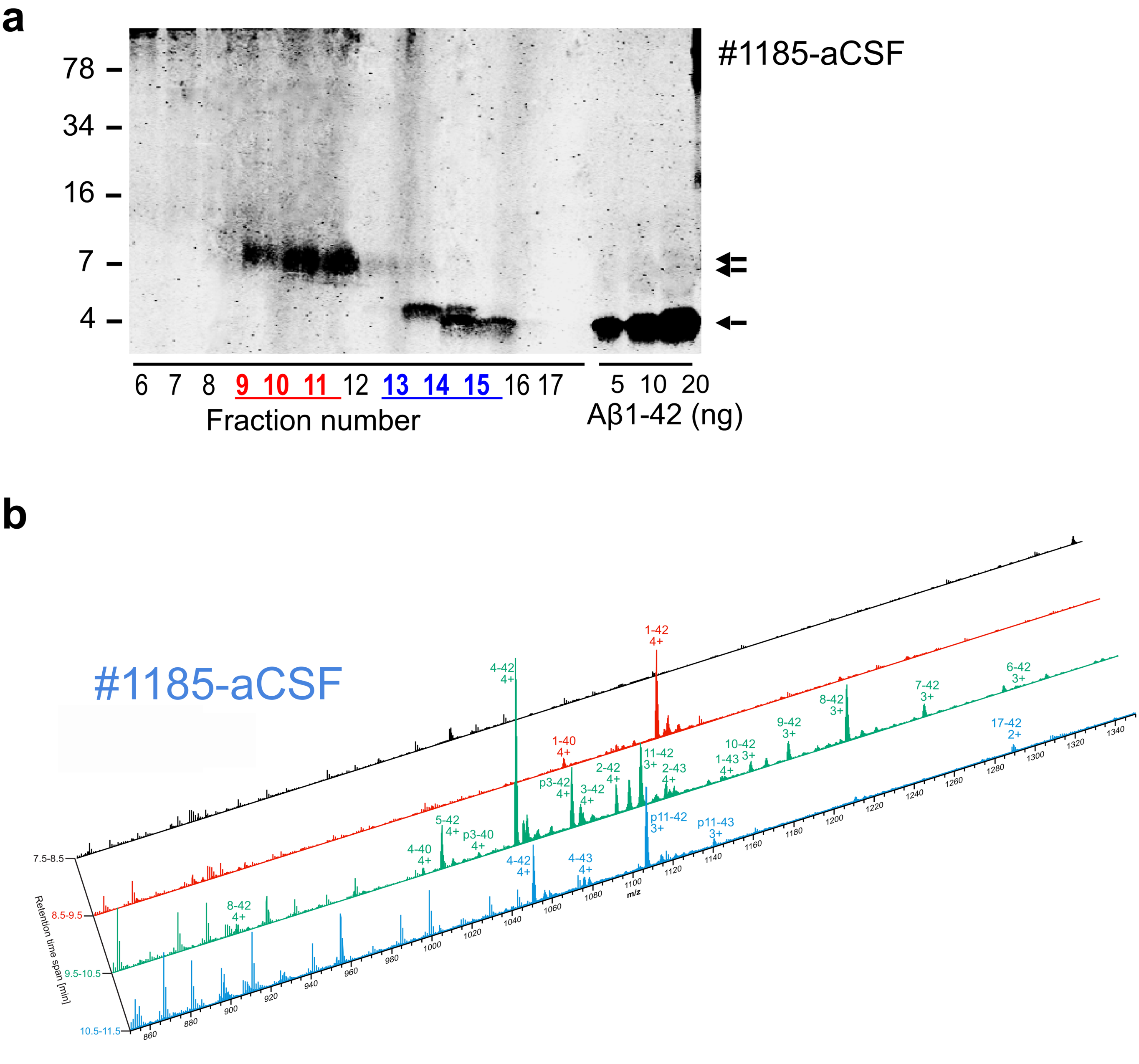
Supplementary Fig. 5



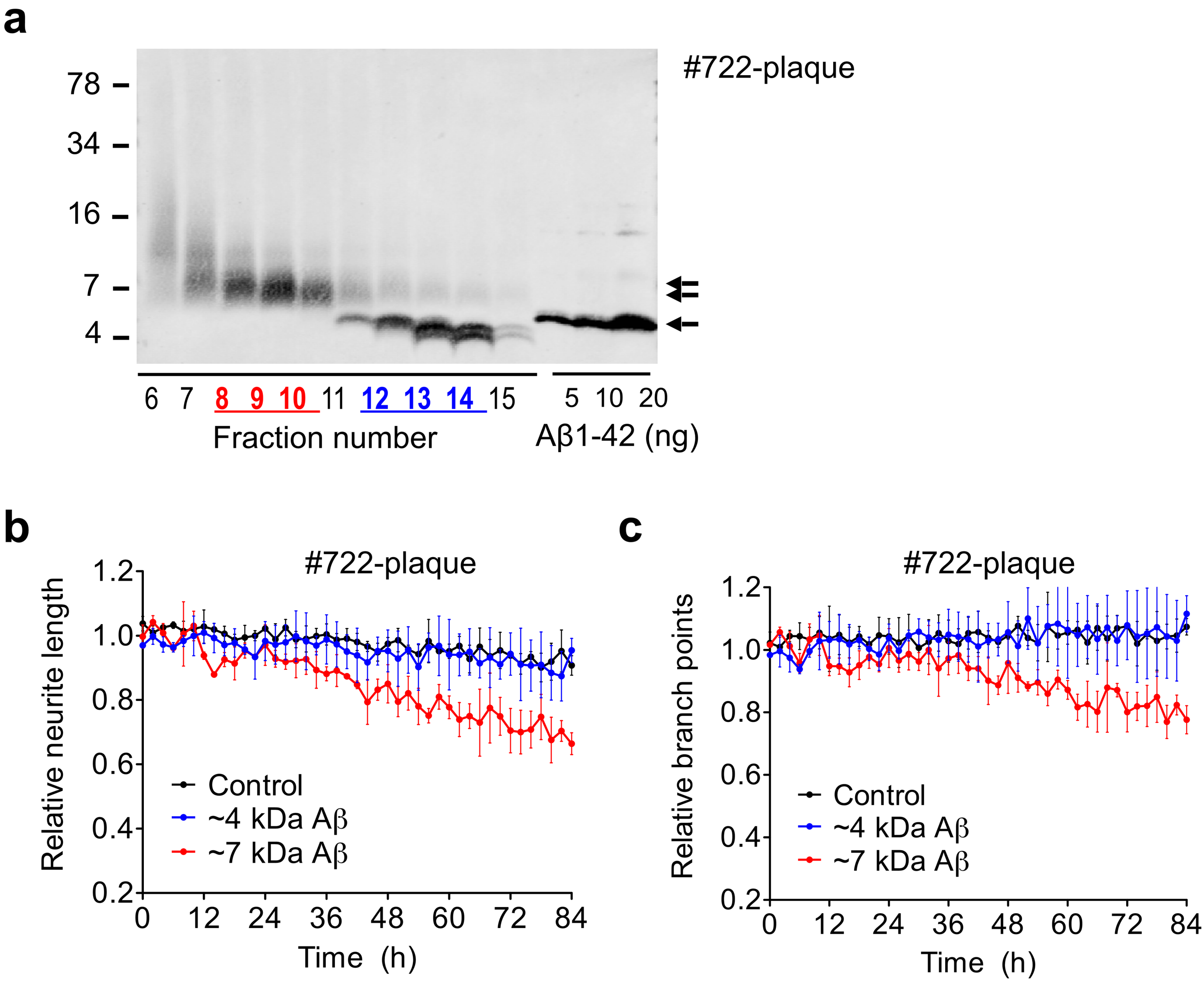




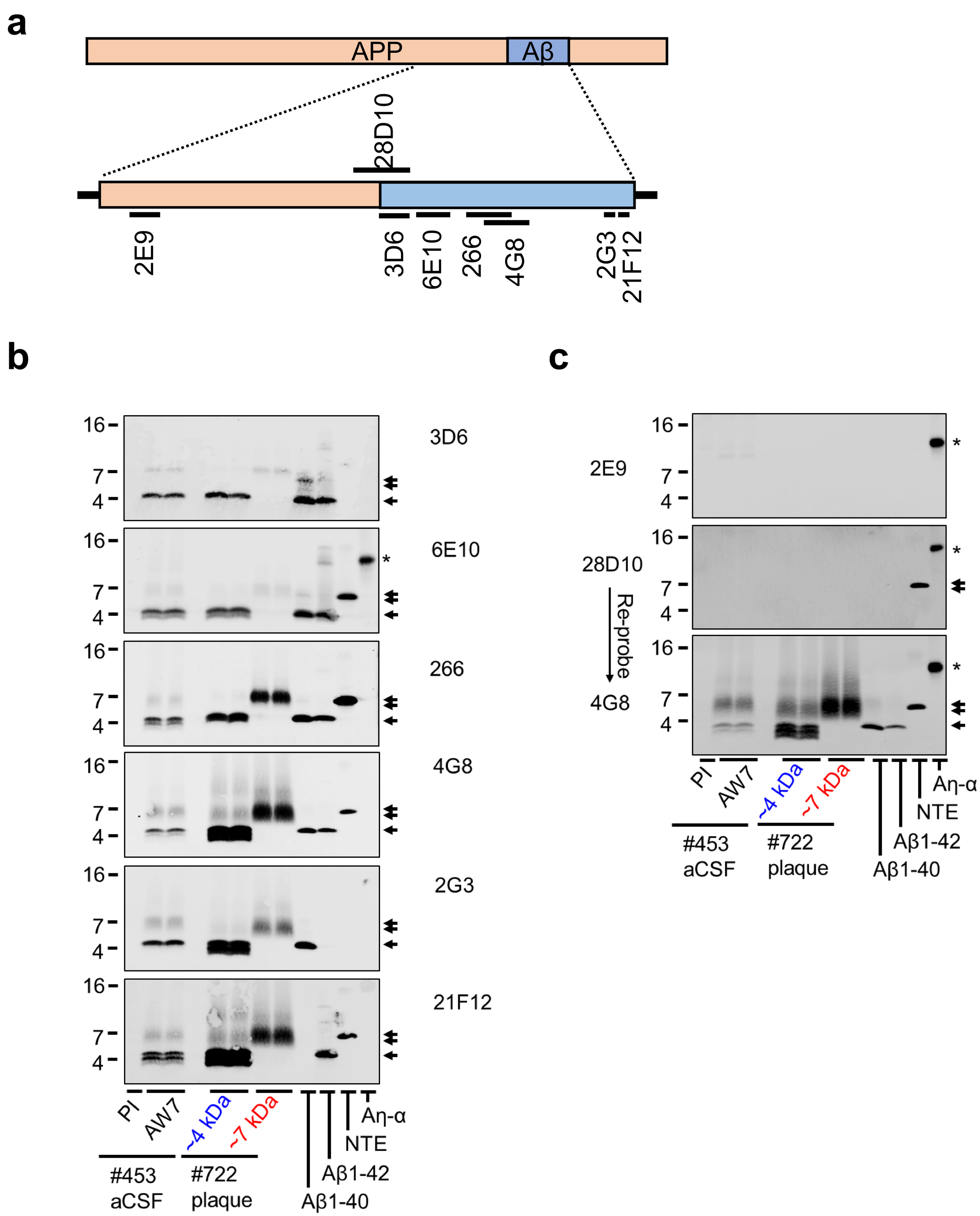
Supplementary Fig. 6



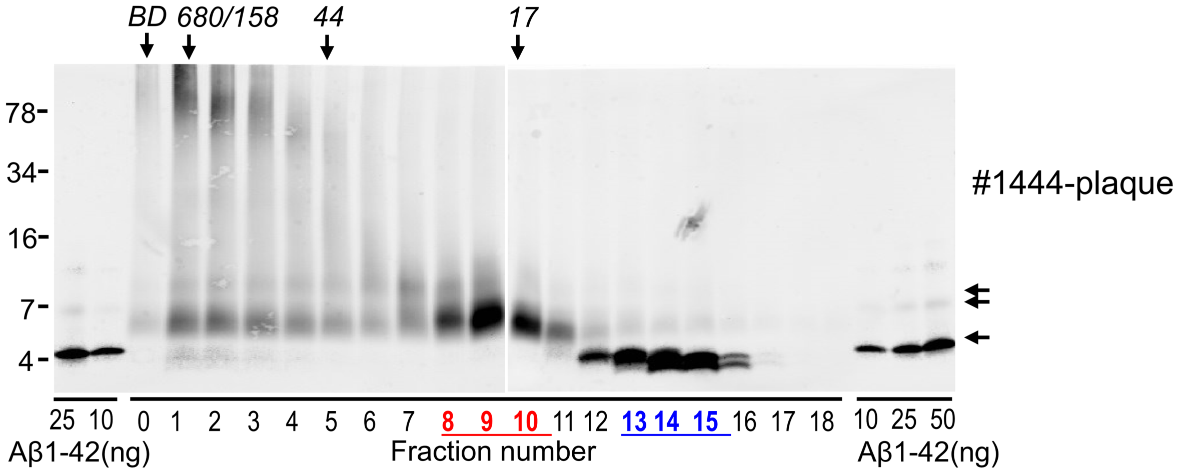
Supplementary Fig. 7



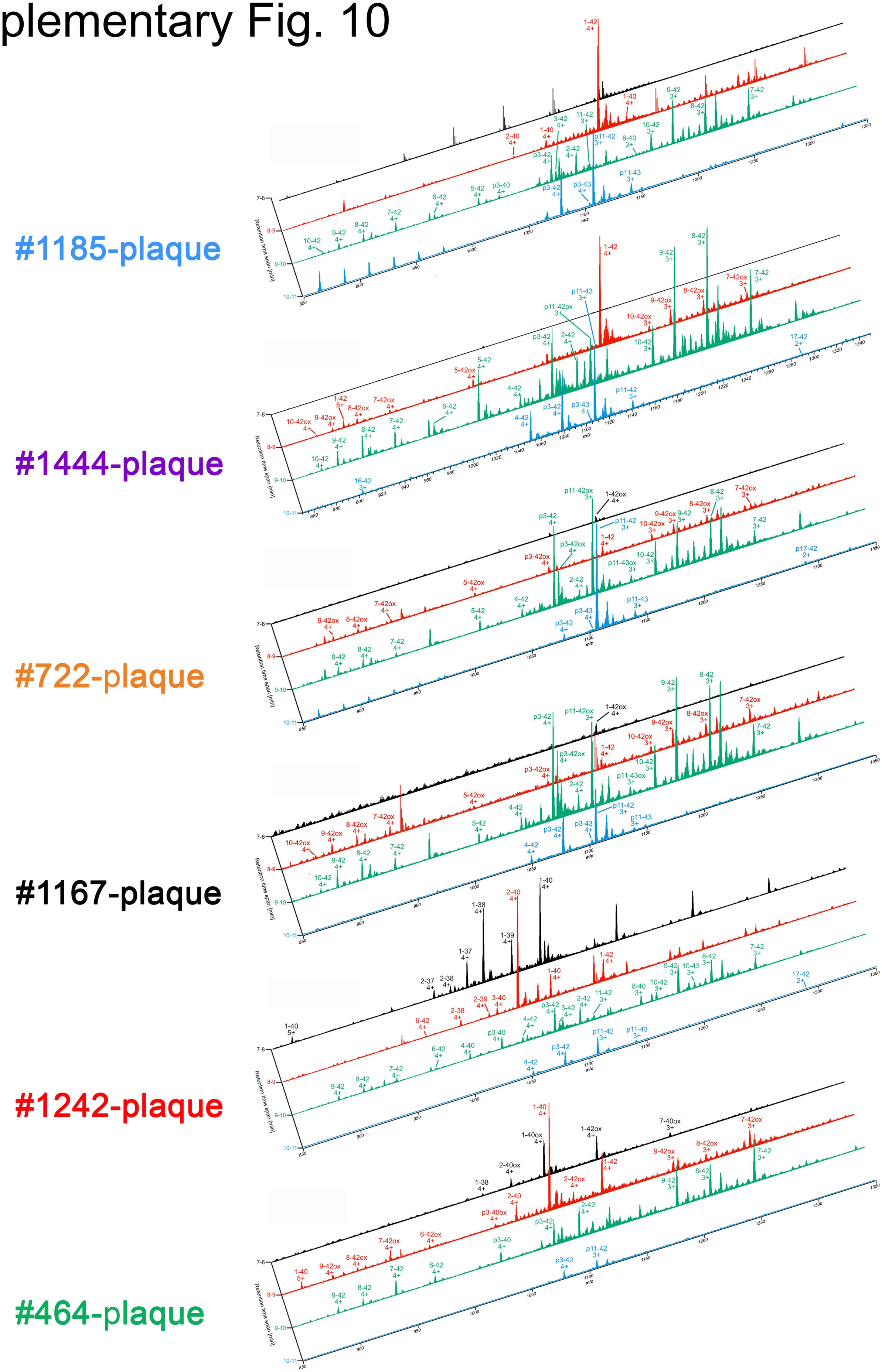
Supplementary Fig. 8



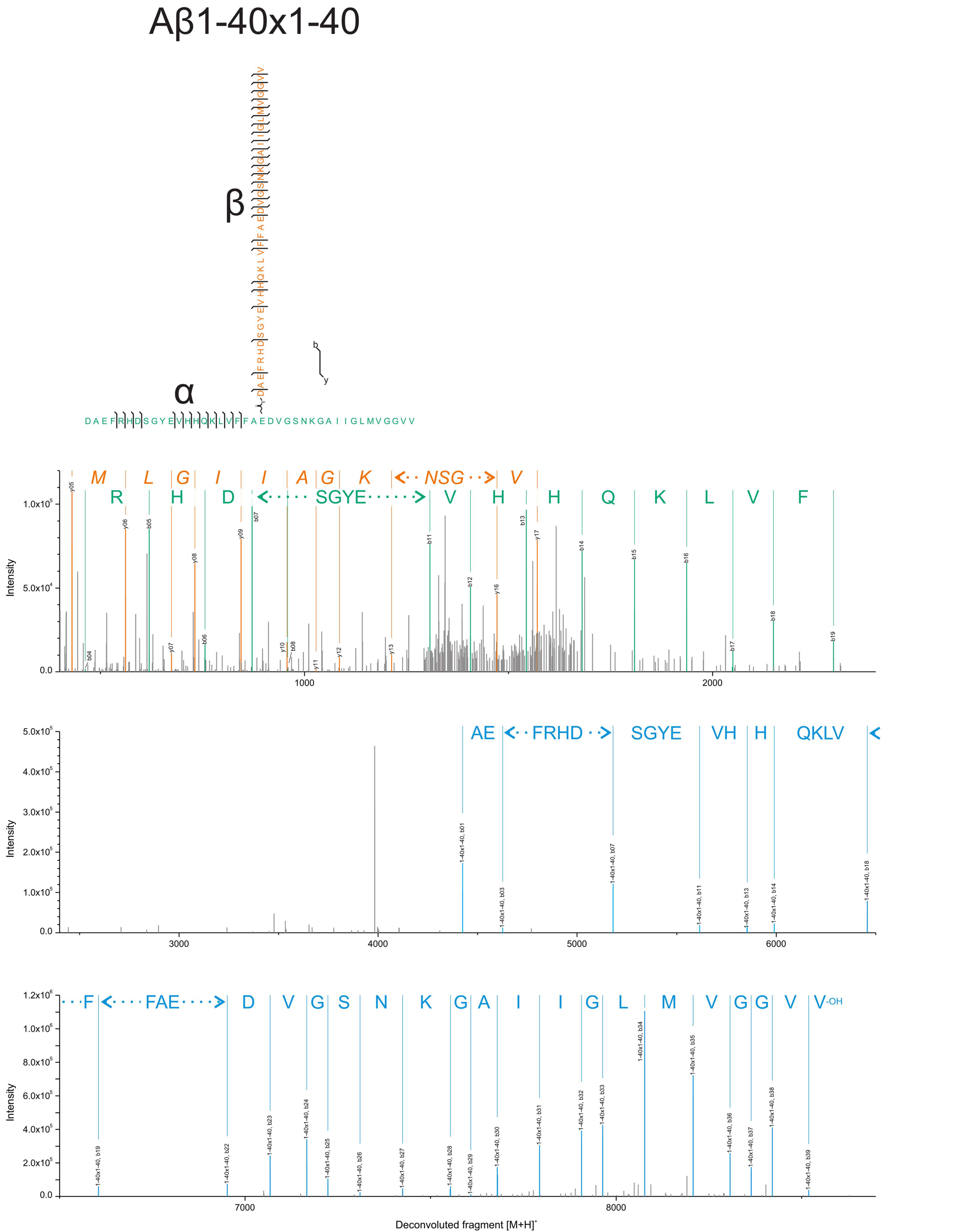
Supplementary Fig. 9



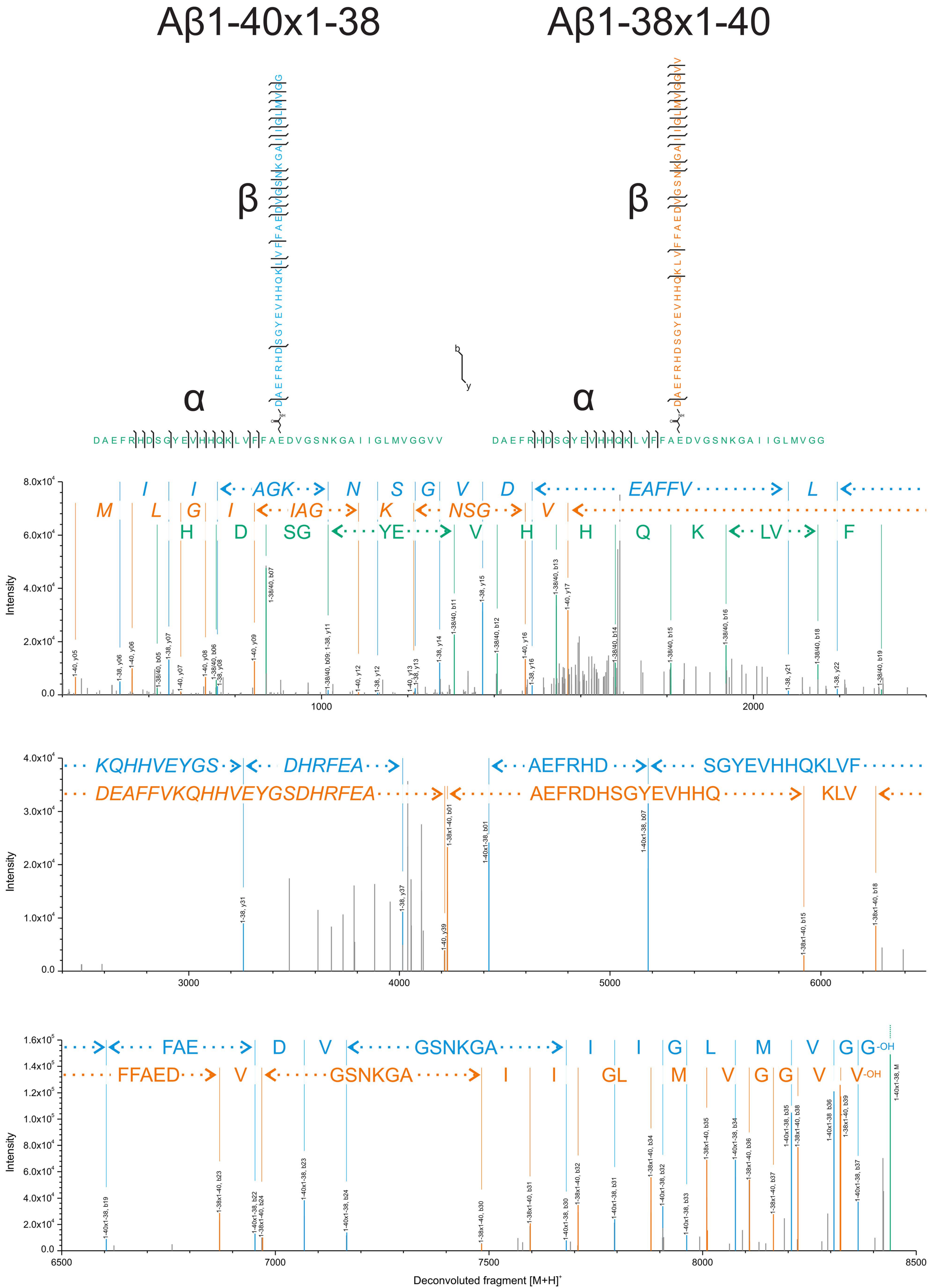
Supplementary Fig. 10



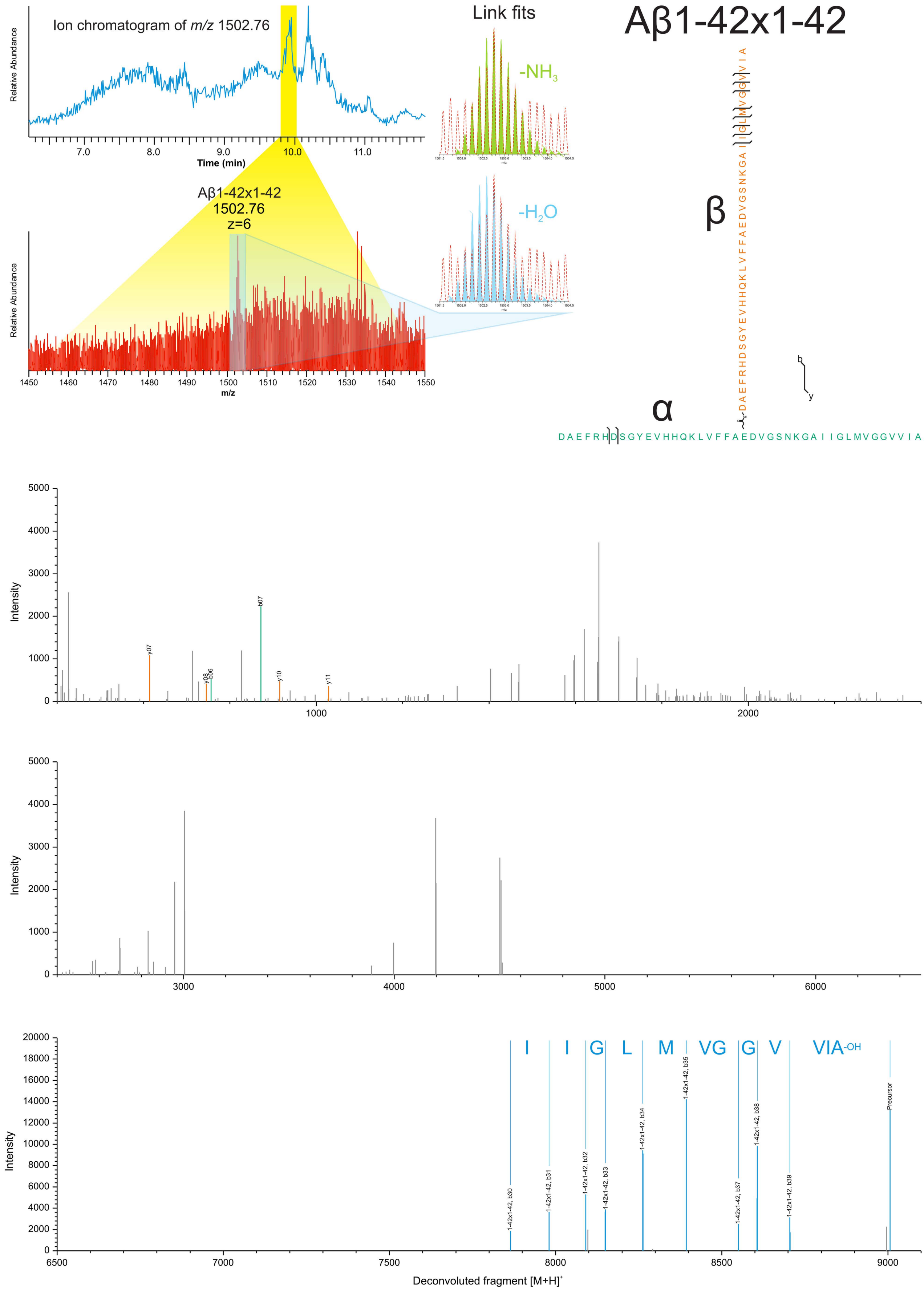
Supplementary Fig. 11



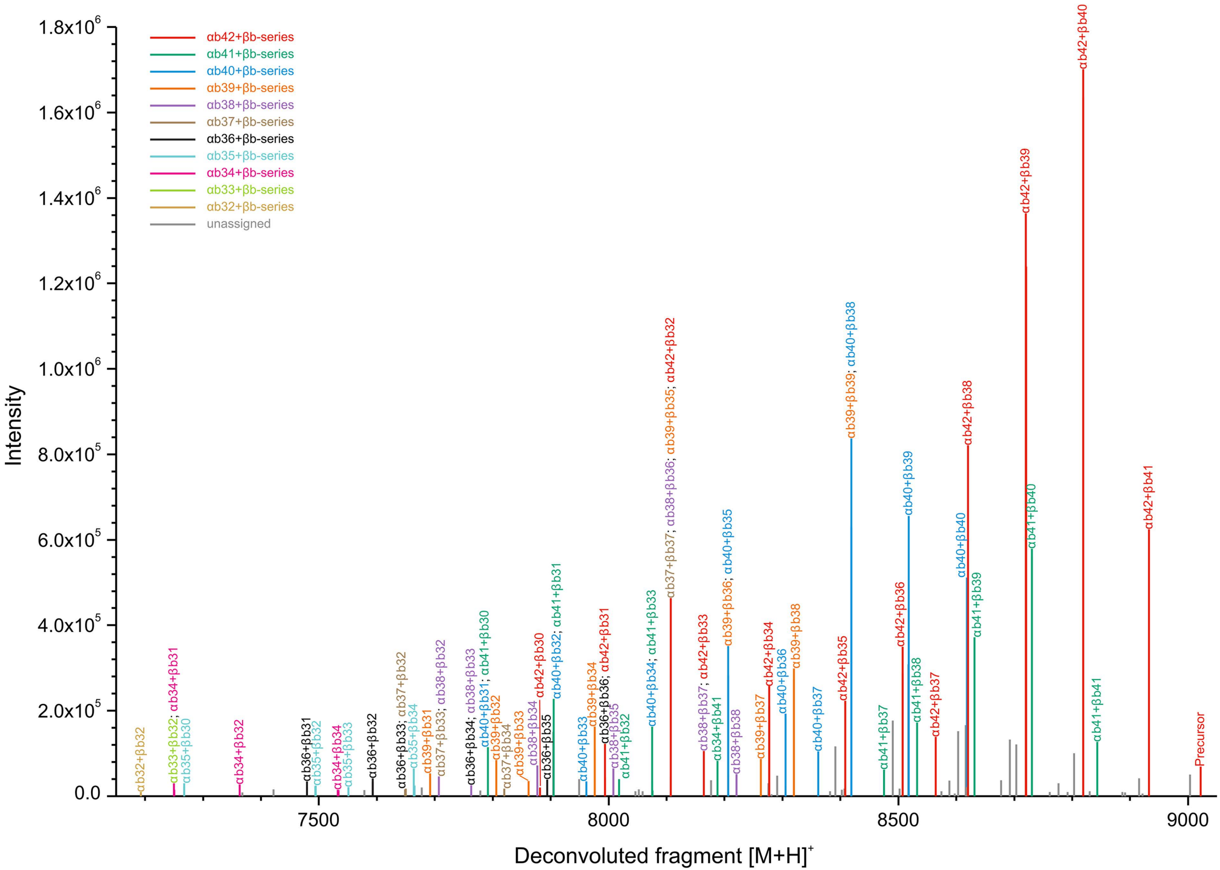
Supplementary Fig. 12



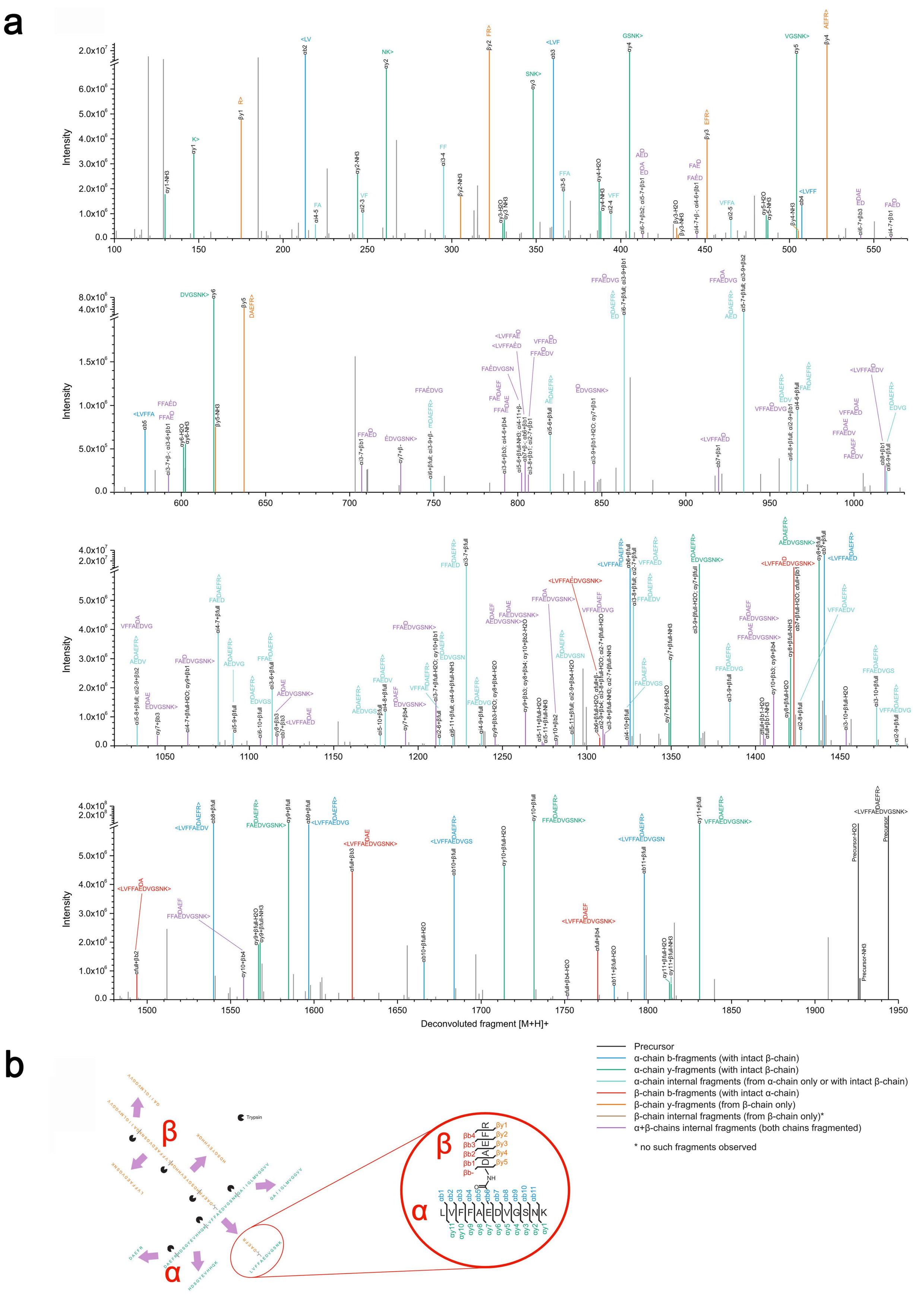
Supplementary Fig. 13



Supplementary Fig. 14



Supplementary Fig. 15



Supplementary Table 1. Aβ species identified by MS/MS using PEAKS Studio of LC-MS/MS from SEC-isolated Aβ monomers. Δm = relative mass deviation between measured and theoretical masses. –10lgP is the PEAKS Studio identification score using the specified settings described in Supplementary information, section *Specific PEAKS Studio 8.5 processing parameters for scores given in Suppl. Table 1*, where 200 is the best value obtainable. The numbers in the respective sample columns are peak areas as determined by PEAKS Studio. All other numbers reflect the best match in the overall dataset.

Sequence	**Peptide**	**Start**	**End**	**Length**	**PTM**	**RT [min]**	**Mass [Da]**	**m/z**	**z**	**Δm [ppm]**	**–10lgP**	**464 M**	**1242 M**	**1167 M**	**722 M**	**1185 M**
DAEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVG	1-37	1	37	37		7.17	4071.9900	1358.3373	3	0.0	200	2.44E+06	1.76E+08			1.64E+06
DAEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLmVG	1-37ox	1	37	37	Mox	6.74	4087.9849	1023.0043	4	0.8	200		1.74E+07			
AEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVG	2-37	2	37	36		7.67	3956.9631	990.2479	4	-0.1	200		7.03E+07			
DAEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGG	1-38	1	38	38		7.30	4129.0117	1377.3442	3	-0.2	200	5.41E+06	7.29E+08			
DAEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLmVGG	1-38ox	1	38	38	Mox	6.73	4145.0063	1037.2585	4	-0.3	200	1.42E+06	5.42E+07			
AEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGG	2-38	2	38	37		7.93	4013.9846	1004.5036	4	0.2	200		7.23E+07			
AEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLmVGG	2-38ox	2	38	37	Mox	7.34	4029.9795	1008.5015	4	-0.7	200		4.94E+07			
DAEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGV	1-39	1	39	39		7.52	4228.0801	1058.0293	4	1.9	200		2.91E+08			
DAEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLmVGGV	1-39ox	1	39	39	Mox	6.92	4244.0747	1062.0261	4	0.2	200		1.25E+07			
AEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGV	2-39	2	39	38		8.28	4113.0527	1029.2778	4	7.2	200		3.51E+07			
DAEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVV	1-40	1	40	40		8.14	4327.1484	1082.7964	4	1.9	200	2.65E+08	9.17E+08		1.66E+06	3.42E+07
DAEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLmVGGVV	1-40ox	1	40	40	Mox	7.39	4343.1431	1448.7229	3	0.9	200	9.61E+07	1.80E+08			2.06E+06
AEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVV	2-40	2	40	39		8.75	4212.1216	1054.0381	4	0.4	200	4.02E+07	6.24E+08			5.34E+06
AEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLmVGGVV	2-40ox	2	40	39	Mox	7.88	4228.1162	1058.0361	4	-0.2	200	1.95E+07	6.58E+07			
EFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVV	3-40	3	40	38		8.69	4141.0845	1036.2799	4	1.5	200		3.74E+07			
eFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVV	p3-40	3	40	38	pE	9.55	4123.0737	1031.7781	4	2.3	200	2.34E+07	9.37E+07			
FRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVV	4-40	4	40	37		9.49	4012.0417	1004.0197	4	1.9	200		4.32E+07			
DSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVV	7-40	7	40	34		8.51	3571.8132	1191.6152	3	3.0	200	5.16E+06	1.07E+07			9.27E+06
DSGYEVHHQKLVFFAEDVGSNKGAIIGLmVGGVV	7-40ox	7	40	34	Mox	7.56	3587.8081	897.9610	4	1.9	200	7.26E+06				
SGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVV	8-40	8	40	33		9.08	3456.7864	1153.2684	3	-0.8	200	2.88E+07	8.27E+07			1.43E+07
SGYEVHHQKLVFFAEDVGSNKGAIIGLmVGGVV	8-40ox	8	40	33	Mox	8.11	3472.7812	1158.6050	3	3.4	200	9.31E+06				
GYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVV	9-40	9	40	32		9.22	3369.7544	1124.2603	3	1.3	200	2.52E+07	5.10E+07			5.26E+06
EVHHQKLVFFAEDVGSNKGAIIGLMVGGVV	11-40	11	40	30		9.00	3149.6694	1050.9004	3	3.1	200		9.45E+06			
eVHHQKLVFFAEDVGSNKGAIIGLMVGGVV	p11-40	11	40	30	pE	9.89	3131.6589	1044.8950	3	1.4	200		1.13E+07			
DAEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIA	1-42	1	42	42		8.56	4511.2695	1504.7668	3	2.0	200	9.55E+07	1.63E+08	6.26E+06	1.47E+07	3.44E+08
DAEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLmVGGVVIA	1-42ox	1	42	42	Mox	7.79	4527.2642	1132.8245	4	1.0	200	5.25E+07	2.91E+07	1.28E+07	2.53E+06	1.23E+08

AEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIA	2-42	2	42	41		9.18	4396.2427	1100.0686	4	0.6	200	8.42E+07	9.20E+07	1.39E+07	1.67E+07	1.20E+08
AEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLmVGGVVIA	2-42ox	2	42	41	Mox	8.41	4412.2373	1104.0691	4	2.3	200	2.28E+07		1.92E+06	3.88E+06	9.78E+06
EFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIA	3-42	3	42	40		9.17	4325.2056	1082.3093	4	0.6	200	1.45E+06	3.75E+01			2.10E+07
eFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIA	p3-42	3	42	40	pE	9.85	4307.1948	1077.8071	4	1.1	200	4.61E+07	1.93E+08	1.14E+08	2.00E+08	3.85E+08
eFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLmVGGVVIA	p3-42ox	3	42	40	pE; Mox	9.13	4323.1899	1081.8057	4	0.8	200	1.28E+07	7.31E+07	6.28E+07	5.69E+07	4.16E+07
FRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIA	4-42	4	42	39		9.90	4196.1631	1050.0486	4	0.5	200	1.26E+06	4.25E+07	2.22E+07	1.58E+07	
FRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLmVGGVVIA	4-42ox	4	42	39	Mox	9.09	4212.1577	1054.0496	4	2.7	200			1.09E+07		
RHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIA	5-42	5	42	38		9.49	4049.0945	1013.2809	4	0.0	200			9.99E+06	1.82E+07	3.08E+07
RHDSGYEVHHQKLVFFAEDVGSNKGAIIGLmVGGVVIA	5-42ox	5	42	38	Mox	8.51	4065.0894	1017.2789	4	-0.7	200			2.42E+06	6.19E+06	
HDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIA	6-42	6	42	37		9.19	3892.9934	974.2577	4	2.1	200	2.49E+07	1.73E+07	8.73E+05		3.73E+07
HDSGYEVHHQKLVFFAEDVGSNKGAIIGLmVGGVVIA	6-42ox	6	42	37	Mox	8.14	3908.9883	978.2529	4	-1.4	200	5.47E+06		3.17E+06	2.85E+06	
DSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIA	7-42	7	42	36		9.07	3755.9343	939.9922	4	1.4	200	3.30E+07	1.41E+08	3.83E+07	3.12E+07	2.06E+08
DSGYEVHHQKLVFFAEDVGSNKGAIIGLmVGGVVIA	7-42ox	7	42	36	Mox	8.09	3771.9294	943.9919	4	2.4	200	5.13E+07		1.97E+07	1.73E+07	1.68E+07
SGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIA	8-42	8	42	35		9.59	3640.9075	1214.6449	3	1.5	200	7.96E+07	2.85E+07	4.29E+07	7.69E+07	6.38E+07
SGYEVHHQKLVFFAEDVGSNKGAIIGLmVGGVVIA	8-42ox	8	42	35	Mox	8.67	3656.9023	915.2333	4	0.5	200	1.75E+07	9.41E+06	2.21E+07	2.30E+07	
GYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIA	9-42	9	42	34		9.71	3553.8755	889.4766	4	0.5	200	2.14E+07	9.17E+07	2.24E+07	1.01E+08	9.29E+07
GYEVHHQKLVFFAEDVGSNKGAIIGLmVGGVVIA	9-42ox	9	42	34	Mox	8.79	3569.8704	893.4760	4	1.3	200	2.26E+07	1.29E+07	2.87E+07	2.27E+07	1.59E+07
YEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIA	10-42	10	42	33		9.75	3496.8540	1166.6282	3	2.5	200	1.16E+07	5.19E+07	4.30E+07	5.77E+07	4.87E+07
YEVHHQKLVFFAEDVGSNKGAIIGLmVGGVVIA	10-42ox	10	42	33	Mox	8.79	3512.8489	1171.9576	3	0.6	200			9.34E+06	1.55E+07	
EVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIA	11-42	11	42	32		9.56	3333.7908	1112.2717	3	0.8	200	5.67E+06	2.40E+07			1.36E+07
EVHHQKLVFFAEDVGSNKGAIIGLmVGGVVIA	11-42ox	11	42	32	Mox	8.76	3349.7856	1117.6028	3	0.3	200					
eVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIA	p11-42	11	42	32	pE	10.41	3315.7800	1106.2695	3	2.0	200	1.59E+07	1.43E+08	5.25E+07	7.46E+07	4.21E+08
eVHHQKLVFFAEDVGSNKGAIIGLmVGGVVIA	p11-42ox	11	42	32	pE; Mox	9.37	3331.7749	1111.6028	3	3.5	200	1.84E+07	1.01E+07	1.00E+08	6.99E+07	1.46E+07
LVFFAEDVGSNKGAIIGLMVGGVVIA	17-42	17	42	26		10.48	2575.4082	1288.7136	2	1.7	200		1.41E+06		3.37E+06	
DAEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIAT	1-43	1	43	43		9.15	4612.3174	1154.0837	4	-2.5	200					2.72E+07
DAEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLmVGGVVIAT	1-43ox	1	43	43	Mox	7.95	4628.3120	1158.0884	4	2.7	137	3.74E+06				
AEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIAT	2-43	2	43	42		9.79	4497.2900	1125.3330	4	2.9	101					
eFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIAT	p3-43	3	43	41	pE	10.07	4408.2427	1103.0696	4	1.5	200	1.28E+06	5.14E+06	3.49E+06	7.42E+06	1.47E+07
FRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIAT	4-43	4	43	40		10.25	4297.2104	1075.3112	4	1.2	200					
DSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIAT	7-43	7	43	37		9.24	3856.9822	1286.6714	3	2.6	135	7.67E+06				
SGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIAT	8-43	8	43	36		9.93	3741.9551	1248.3276	3	1.6	200		6.64E+06			
GYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIAT	9-43	9	43	35		9.84	3654.9231	1219.3174	3	2.0	151		7.02E+06	4.86E+06		2.03E+07
eVHHQKLVFFAEDVGSNKGAIIGLMVGGVVIAT	p11-43	11	43	33	pE	10.48	3416.8279	1139.9517	3	1.5	200	1.69E+06	1.54E+07	1.98E+06	1.20E+07	3.87E+07
eVHHQKLVFFAEDVGSNKGAIIGLmVGGVVIAT	p11-43ox	11	43	33	pE; Mox	9.36	3432.8228	1145.2811	3	-0.3	200			8.36E+06	1.26E+07	

Supplementary Table 2. MS/MS-identified cross-linked Aβ in SEC-isolated ~7 kDa Aβ from brain #1242. PEAKS Studio and Xtract were used to deconvolute LC-MS/MS spectra; all peaks were then evaluated manually. [a]Δm = relative mass deviation between measured and theoretical masses; [b] * denotes scans presented in Supplementary Figs. 11 and 12; [c] –10lgP is the PEAKS Studio identification score using the specified settings described in Supplementary information, section *Specific PEAKS Studio 8.5 processing parameters for scores given in Supplementary Table 2*, missing value = no score determined.

Dimer (α×β)	m/z	Charge	Exp. mass [Da]	Theor. mass -18 link [Da]	Δm[a] [ppm]	Δm [Da]	RT [min]	Scan[b]	–10lgP[c]	α-chain only b-ions	y-ions	α×β-chains b-ions
1-37×1-38 + 1-38×1-37	1364.834	6	8182.963	8182.991	-3.4	-0.03	10.0795	1484	6.73	6	4 + 3	7 + 5
1-38×1-38	1374.169	6	8238.970	8240.013	-126.5	-1.04	10.1658	1494	15.84	3	3	14
1-38×1-38	1649.007	5	8239.999	8240.013	-1.7	-0.01	10.1968	1498		3	2	4
1-38×1-39 + 1-39×1-38	1391.021	6	8340.082	8339.081	120.0	1.00	10.2804	1508	10.47	3	4 + 3	7 + 6
1-37×1-40 + 1-40×1-37	1397.856	6	8381.092	8381.128	-4.3	-0.04	10.339	1515	16.79	7	6 + 6	11 + 13
1-37×1-40 + 1-40×1-37	1198.164	7	8380.097	8381.128	-123.1	-1.03	10.3949	1522	15.83	7	4 + 3	8 + 6
1-37×1-40 + 1-40×1-37	1397.853	6	8381.077	8381.128	-6.1	-0.05	10.4258	1526	20.71	5	6 + 6	8 + 8
1-38×1-40 + 1-40×1-38	1407.357	6	8438.096	8438.149	-6.3	-0.05	10.3672	1519	11.13	6	6 + 6	7 + 8
1-38×1-40 + 1-40×1-38	1688.636	5	8438.144	8438.149	-0.7	-0.01	10.4442	* 1528	23.29	12	10 + 13	14 + 14
1-38×1-40 + 1-40×1-38	1206.451	7	8438.109	8438.149	-4.8	-0.04	10.4535	1529	24.37	9	4 + 4	15 + 14
1-38×1-40 + 1-40×1-38	1407.354	6	8438.083	8438.149	-7.8	-0.07	10.4844	1533	24.00	12	6 + 6	20 + 16
1-38×1-40 + 1-40×1-38	1688.838	5	8439.153	8438.149	118.9	1.00	10.5403	1540		3	5 + 5	3 + 2
1-39×1-40 + 1-40×1-39	1423.872	6	8537.191	8537.218	-3.2	-0.03	10.5213	1537	14.62	3	7 + 4	8 + 7
1-39×1-40 + 1-40×1-39	1708.445	5	8537.187	8537.218	-3.7	-0.03	10.5772	1544	21.80	8	7 + 5	9 + 10
1-39×1-40 + 1-40×1-39	1423.874	6	8537.198	8537.218	-2.4	-0.02	10.5989	1547	22.10	11	6 + 6	15 + 15
1-39×1-40 + 1-40×1-39	1220.753	7	8538.217	8537.218	117.0	1.00	10.6174	1549		4	4 + 3	5 + 6
1-40×1-40	1440.549	6	8637.250	8636.286	111.6	0.96	10.676	1556	26.95	8	9	19
1-40×1-40	1234.760	7	8636.271	8636.286	-1.8	-0.02	10.7319	1563	27.25	12	7	23
1-40×1-40	1440.389	6	8636.288	8636.286	0.2	0.00	10.7721	* 1568	28.92	13	11	26
1-40×1-40	1728.261	5	8636.270	8636.286	-1.9	-0.02	10.7906	1570	28.47	13	15	17
1-40×1-40	1080.546	8	8636.307	8636.286	2.4	0.02	10.7998	1571	20.66	5	5	14
1-40×1-40	1234.472	7	8634.255	8636.286	-235.2	-2.03	10.8279	1575		4	6	13
1-40×1-40	1440.383	6	8636.252	8636.286	-4.0	-0.03	10.8866	1582	14.02	4	6	8
2-38×1-40 + 2-40×1-38	1388.360	6	8324.116	8323.122	119.4	0.99	10.7411	1564	23.58	8	5 + 3	11 + 8
2-40×1-40	1705.455	5	8522.238	8521.259	114.8	0.98	10.6945	1558	15.63	1	9	8
2-40×1-40	1421.384	6	8522.259	8521.259	117.3	1.00	10.9729	1592	19.13	5	7	10
2-40×1-40	1705.653	5	8523.228	8521.259	231.0	1.97	11.038	1600		6	9	14
2-40×1-40	1421.215	6	8521.246	8521.259	-1.5	-0.01	11.0597	1603	26.06	11	7	24
2-40×1-40	1218.322	7	8521.205	8521.259	-6.4	-0.05	11.0966	1607	15.68	3	4	7
1-40×1-42 + 1-42×1-40	1471.072	6	8820.387	8820.407	-2.3	-0.02	11.0288	1599		2	2 + 4	6 + 4

Supplementary Table 3

Peak list for Suppl. Fig. 11 Aβ1-40×1-40; $-H_2O$ link Scan 1568 Charge 6+ Selected m/z 1440.3887 RT 10.77 min					
Experimental $[M+H]^+$ [Da]	Intensity	Fragment label	Theoretical $[M+H]^+$ [Da]	Δm [ppm]	Δm [Da]
401.2173	28810				
401.2173	36169				
401.2207	36573				
402.1796	1498				
412.2546	15324				
413.2209	2604				
415.2364	10897				
416.1956	8130				
416.1973	7471				
416.1973	7471				
416.2273	35057				
416.2273	27935				
416.2314	36026				
422.2395	1960				
430.2473	9836				
430.2481	8194				
430.2652	107362				
430.2673	74399				
430.2673	107362	y05	430.2666	1.7	0.0007
438.2701	1995				
438.3071	1893				
444.2266	59886				
444.2273	42941				
444.2273	57340				
455.2673	1327				
458.2421	17140				
463.1815	1899	b04	463.1829	-3.0	-0.0014
469.2833	4446				
483.2921	2500				
483.3273	2619				
483.3273	2619				
483.3276	2653				

484.2862	592				
484.3302	303				
486.3096	6125				
487.2693	13101				
497.2529	2375				
497.2573	2459				
497.2573	2459				
498.2559	601				
498.2730	1110				
501.2484	854				
504.2559	1866				
507.3021	927				
512.2888	2311				
514.3048	16922				
515.2638	33764				
515.2673	35049				
515.3068	1712				
516.2673	5406				
521.3070	2592				
525.3386	4650				
526.3047	1639				
528.3214	1564				
529.2789	2502				
529.3163	5046				
538.3337	972				
540.3495	5425				
542.3278	1558				
543.2933	5260				
543.3308	943				
556.2623	3275				
557.3073	7096				
557.3073	8920				
557.3107	8799				
561.3057	84485				
561.3073	85163	y06	561.3070	0.4	0.0002
561.3073	44916				
568.3503	951				
569.3099	5858				
571.3210	5910				
586.3368	34384				
586.3373	33376				

586.3373	18433				
596.3173	20240				
596.3217	20193				
596.3682	2602				
597.3712	1520				
599.3558	1835				
600.3527	5087				
601.3534	86				
606.3700	1340				
610.3361	1654				
611.3135	981				
614.3273	70646				
614.3273	32676				
614.3317	69971				
615.3345	1667				
619.2773	11621	b05	619.2840	-10.9	-0.0067
619.2773	7519				
619.2819	11590				
627.3883	5431				
628.3442	22380				
634.3903	1060				
638.3668	1077				
642.3626	1846				
647.6424	909				
653.4333	15014				
653.4373	15713				
654.3912	2470				
656.3773	3903				
656.3773	7549				
656.3781	6754				
657.3804	1041				
674.3873	11545	y07	674.3911	-5.7	-0.0038
674.3873	5702				
674.3886	11017				
675.3916	1077				
682.3925	1304				
684.4063	1781				
685.3611	1433				
685.4093	1008				
687.3180	920				
688.2940	921				

689.8041	1696				
690.8071	1052				
699.4173	6796				
699.4173	12642				
699.4200	12420				
703.7973	7129				
704.8038	1497				
709.4050	3723				
713.3997	3122				
727.4138	35839				
727.4173	34939				
728.4173	8741				
731.4073	22788				
731.4073	64907	y08	731.4126	-7.2	-0.0053
731.4102	64615				
741.4250	19247				
741.4273	17307				
741.4273	8681				
755.4470	8156				
755.4473	8531				
755.4473	4098				
756.3373	7186				
756.3373	16216				
756.3401	16455	b06	756.3429	-3.7	-0.0028
758.3273	7142				
767.4760	6736				
772.8312	4250				
781.4193	1577				
784.4287	2118				
784.4725	11740				
786.4793	231				
798.4426	9810				
812.4668	3747				
818.8629	2632				
826.8573	3456				
827.8643	867				
838.7336	958				
840.4944	23151				
841.3601	3982				
841.4973	7375				
844.4937	77755				

844.4973	79386	y09	844.4966	0.8	0.0006
845.4973	5608				
848.3785	1139				
850.8744	1149				
854.3400	1508				
854.5066	6797				
859.4177	1092				
869.4893	2967				
871.3668	100160				
871.3673	103557	b07	871.3698	-3.0	-0.0026
883.5367	8444				
891.3918	1814				
896.3770	1317				
897.5073	13961				
897.5123	11088				
898.5147	3802				
898.5173	6492				
905.3895	5024				
905.8909	878				
909.7969	1028				
911.5273	29982				
911.5273	6608				
911.5281	28120				
912.5331	2672				
934.7658	1337				
940.5621	7000				
956.5215	1078				
957.5773	4821				
957.5773	17426				
957.5777	17786	y10	957.5807	-3.1	-0.0030
958.3955	1380	b08	958.4019	-6.7	-0.0064
958.5801	2256				
958.9600	1814				
959.9630	569				
960.4226	2700				
967.9640	1034				
968.5573	8884				
970.5602	1828				
972.5357	1087				
973.4885	1400				
985.5469	7937				

985.5473	7748				
997.5773	11647				
997.5819	11689				
1008.9624	965				
1010.5967	28667				
1010.5973	6779				
1010.5973	28361				
1028.6113	1581	y11	1028.6178	-6.3	-0.0065
1029.0550	93				
1042.5681	23983				
1043.5673	12603				
1043.5703	790				
1044.5737	2062				
1045.5732	362				
1056.9355	1293				
1060.4573	981				
1060.5413	1118				
1061.5161	1189				
1075.0073	5284				
1084.5675	2366				
1084.6116	2189				
1085.6326	8796	y12	1085.6393	-6.1	-0.0067
1091.5327	2100				
1096.6534	2117				
1107.6167	2434				
1111.6262	3340				
1125.6173	14070				
1125.6216	14026				
1141.6353	35687				
1142.6373	18403				
1151.9194	3709				
1162.2437	4978				
1179.1249	5545				
1180.5873	7551				
1195.9712	4895				
1198.6580	20742				
1199.5754	6235				
1199.5773	5873				
1199.6573	9576				
1200.5773	6882				
1213.7273	10623	y13	1213.7342	-5.7	-0.0070

1213.7288	9464				
1219.6173	5342				
1240.7073	8691				
1250.5973	13069				
1253.9473	8284				
1255.6773	33702				
1255.6800	30648				
1293.2373	14334				
1294.6373	7407				
1294.9773	7060				
1295.1473	4774				
1297.1273	8684				
1299.8073	12239				
1303.6273	14779				
1307.5251	20262				
1307.5373	76241	b11	1307.5293	6.1	0.0080
1307.6373	12809				
1307.9673	7610				
1309.1573	9000				
1309.6473	6759				
1309.8073	12552				
1311.3073	12583				
1311.6473	8387				
1313.9773	11431				
1315.3273	8767				
1318.9873	13850				
1319.6573	13447				
1319.8173	6387				
1320.9873	6269				
1322.1473	15185				
1322.6573	22271				
1324.3173	5609				
1326.4873	19656				
1328.6573	57621				
1329.3273	30387				
1330.6673	10903				
1332.9973	11960				
1336.4973	8491				
1336.6473	14435				
1337.8273	16789				
1337.9973	6671				

1339.4873	11903				
1339.8373	10915				
1341.8273	24781				
1342.1573	12123				
1344.3373	53241				
1344.6673	93029				
1349.9973	21705				
1352.6673	24470				
1354.7473	32089				
1355.4973	9960				
1356.6673	17738				
1358.1673	18124				
1358.5073	8498				
1358.8273	11906				
1359.3373	12588				
1361.5073	12424				
1361.8373	16422				
1368.1773	18357				
1373.8473	18601				
1377.1773	11767				
1378.3373	7808				
1380.8473	9609				
1381.0173	11527				
1381.1873	15978				
1384.3473	13670				
1385.8573	40580				
1386.0173	31830				
1388.1873	9075				
1388.8573	18812				
1389.0173	8946				
1391.1873	8441				
1391.8773	11251				
1392.6773	15169				
1393.1973	13038				
1393.5273	14277				
1396.8573	15592				
1397.6873	19322				
1399.0273	10921				
1399.1873	15639				
1399.8573	8367				
1406.5873	50724	b12	1406.5977	-7.4	-0.0104

1406.5935	20440				
1411.2873	11279				
1413.2073	7907				
1415.6773	18078				
1418.3773	11716				
1420.6973	8200				
1422.6873	12815				
1429.7073	16948				
1433.9073	19139				
1437.7173	36535				
1438.0473	39459				
1441.0473	14752				
1446.4973	10712				
1449.1173	6616				
1453.8173	8462				
1460.7073	6708				
1464.6973	22847				
1468.7173	12203				
1469.1273	8408				
1470.5073	8342				
1470.7173	17746				
1471.1273	11731				
1471.8273	46336	y16	1471.8307	-2.3	-0.0034
1473.5173	7658				
1474.3073	7376				
1476.7273	9986				
1481.9073	7212				
1484.5073	7330				
1486.3173	13325				
1486.9173	15822				
1488.3173	11058				
1488.7173	12635				
1489.5173	7315				
1496.1273	7301				
1502.7273	9480				
1507.9273	15669				
1508.1373	13061				
1511.3473	12212				
1512.9373	8631				
1514.7473	15835				
1515.5373	8788				

1515.6558	16561				
1515.6573	9269				
1517.9373	15321				
1519.7473	12386				
1520.9473	9538				
1522.7473	10009				
1523.5473	11236				
1525.1473	9771				
1526.5473	13593				
1526.7373	22109				
1528.1473	11721				
1532.7473	20896				
1533.9473	12891				
1536.5573	13117				
1539.7473	9556				
1543.6473	10127				
1543.6473	96616	b13	1543.6566	-6.0	-0.0093
1543.6514	62798				
1547.7573	12517				
1553.5673	14944				
1555.1673	8433				
1555.3673	9918				
1557.7573	8613				
1557.9573	12479				
1558.1573	24988				
1558.3573	13595				
1559.7673	65997				
1562.7573	21629				
1564.5573	9547				
1564.9673	12327				
1565.3673	9683				
1565.6800	2719				
1565.7673	11392				
1567.3773	13830				
1567.5673	15517				
1568.1773	22791				
1570.5673	51048				
1570.8973	78875	y17	1570.8991	-1.1	-0.0018
1570.9773	23946				
1572.7873	22964				
1575.5673	11520				

1575.9773	23997				
1578.9773	12703				
1580.1773	9218				
1580.3773	9095				
1580.5773	21453				
1580.7673	13323				
1587.0273	28122				
1592.7873	22317				
1599.7873	24583				
1601.9873	16172				
1602.1973	21918				
1603.7973	20197				
1606.7873	9021				
1607.9973	17376				
1608.7973	35915				
1609.1873	14670				
1609.3973	12082				
1611.8073	19892				
1612.9973	13598				
1616.7973	86942				
1622.8173	15559				
1624.6073	7928				
1624.7973	37521				
1624.9973	12692				
1628.7873	24484				
1631.8073	14371				
1634.0073	34190				
1635.5973	11738				
1637.8073	13008				
1640.8073	25833				
1647.6073	8528				
1647.8073	10006				
1651.0273	17023				
1652.7128	15862				
1652.7173	9909				
1653.7177	1702				
1653.8073	20719				
1654.0073	12751				
1659.8273	19016				
1661.0473	18604				
1668.8373	12323				

1677.8173	24728				
1680.7073	39281				
1680.7094	72197	b14	1680.7155	-3.6	-0.0061
1686.8242	56521				
1705.8473	14834				
1706.0373	22677				
1749.8573	16077				
1760.8773	11718				
1803.3899	12846				
1808.7673	9623				
1808.7673	35661				
1808.7682	67087	b15	1808.7741	-3.3	-0.0059
1821.8330	6873				
1829.1260	8012				
1856.6444	9655				
1859.6869	5920				
1866.8851	8201				
1883.9288	7110				
1888.4369	5411				
1892.9307	13267				
1905.9109	7770				
1920.6826	9253				
1921.6952	7449				
1936.8573	37430				
1936.8608	64960	b16	1936.8690	-4.3	-0.0082
1948.9291	6975				
1949.4606	8860				
1977.4664	7032				
1977.9786	12120				
2010.0087	3562				
2019.4836	4074				
2020.0104	429				
2031.9354	21801				
2031.9373	11720				
2048.3720	2934				
2049.9468	12405	b17	2049.9531	-3.1	-0.0063
2052.2559	409				
2054.0107	2298				
2055.0945	4002				
2090.4200	4126				
2100.0352	3071				

2133.7607	4754				
2149.0137	30478	b18	2149.0215	-3.6	-0.0078
2149.0173	18375				
2150.0188	3517				
2163.1016	3449				
2177.4648	4187				
2179.1274	3355				
2204.0952	3727				
2212.5894	11956				
2214.5942	6193				
2296.0773	8790				
2296.0815	18227	b19	2296.0899	-3.7	-0.0084
2313.1316	5142				
2314.6240	3527				
2444.1387	14007				
2444.1473	8151				
2708.3373	13762				
2837.3873	7783				
2897.4873	18439				
3241.5873	13396				
3369.6353	3673				
3452.7397	4340				
3476.6814	39715				
3477.1724	47314				
3534.6921	29471				
3538.7334	9177				
3652.8073	15426				
3652.8203	20613				
3668.8220	13321				
3776.8499	12671				
3866.3673	6270				
3898.9073	6545				
3928.9173	6475				
3982.9487	464348				
3983.4468	326735				
3996.9626	14499				
4000.9573	10565				
4003.4473	5715				
4104.5195	12881				
4106.0107	12099				
4310.1180	5433				

4425.1373	102844				
4425.1520	173756	1-40x1-40, b01	4425.1726	-4.7	-0.0206
4625.2373	12577	1-40x1-40, b03	4625.2523	-3.3	-0.0151
4769.8573	10485				
5180.4920	122069	1-40x1-40, b07	5180.5077	-3.0	-0.0157
5180.4973	105036				
5615.6445	19174	1-40x1-40, b11	5616.6669	-182.1	-1.0224
5852.7930	10868	1-40x1-40, b13	5852.7945	-0.2	-0.0015
5853.7673	17190				
5989.8273	23436	1-40x1-40, b14	5989.8534	-4.4	-0.0261
6458.1340	78917	1-40x1-40, b18	6458.1594	-3.9	-0.0254
6458.1373	35928				
6605.2073	59845	1-40x1-40, b19	6605.2278	-3.1	-0.0205
6934.3173	5651				
6952.3073	75705	1-40x1-40, b22	6952.3759	-9.9	-0.0686
7050.3673	34517				
7050.3880	16503				
7067.3735	244035	1-40x1-40, b23	7067.4029	-4.2	-0.0294
7067.3973	149283				
7121.4173	5571				
7149.4073	16645				
7166.4500	341295	1-40x1-40, b24	7166.4713	-3.0	-0.0213
7166.4573	193184				
7223.4730	106157	1-40x1-40, b25	7223.4927	-2.7	-0.0197
7223.4973	62782				
7293.4773	11445				
7309.4973	25868	1-40x1-40, b26	7310.5246	-140.5	-1.0273
7407.5273	8735				
7424.5420	49326	1-40x1-40, b27	7424.5677	-3.5	-0.0257
7424.5473	41894				
7425.5220	8590				
7478.6073	7591				
7517.6473	7975				
7552.7173	41205	1-40x1-40, b28	7552.6627	7.2	0.0546
7553.6455	59837				
7576.6773	11700				
7608.6673	13523	1-40x1-40, b29	7609.6840	-133.6	-1.0167
7634.6773	15209				
7650.8673	19611				
7664.6773	15872				
7677.7273	8649				

7679.7010	174614				
7680.7173	129642	1-40x1-40, b30	7680.7212	-0.5	-0.0040
7690.6973	14456				
7720.7673	13325				
7734.7473	10283				
7742.7573	4783				
7746.7773	19316				
7753.7673	7045				
7763.7973	8201				
7765.8573	30556				
7776.7573	37773				
7793.7793	308297	1-40x1-40, b31	7793.8053	-3.3	-0.0260
7793.8173	256730				
7796.7660	8083				
7850.8073	16300				
7862.8273	7555				
7863.8373	19139				
7878.7873	22500				
7889.8673	47506				
7894.8773	7472				
7906.8584	393891	1-40x1-40, b32	7906.8894	-3.9	-0.0310
7906.8773	331150				
7936.8673	10652				
7945.8873	67513				
7963.8857	354514				
7963.9173	427188	1-40x1-40, b33	7963.9108	0.8	0.0065
7964.8873	7013				
7965.8965	6927				
7977.8773	23544				
7991.8873	6278				
8001.9073	7721				
8020.9473	33419				
8032.9873	15415				
8034.9373	12019				
8048.9473	82637				
8059.9473	70568				
8076.0150	5426				
8076.9473	859792				
8076.9630	1106595	1-40x1-40, b34	8076.9949	-3.9	-0.0319
8077.9750	5983				
8093.9373	72006				

8133.0573	22323				
8134.9473	11600				
8148.0273	12892				
8176.0073	11647				
8177.9973	20725				
8191.0073	122563				
8208.0080	723106	1-40x1-40, b35	8208.0354	-3.3	-0.0274
8208.0173	589934				
8250.0473	16419				
8261.0373	3739				
8264.9973	13682				
8279.0873	8679				
8290.1073	20052				
8291.0473	18454				
8307.0640	258064	1-40x1-40, b36	8307.1038	-4.8	-0.0398
8307.0773	237448				
8347.0973	13745				
8364.0850	174861	1-40x1-40, b37	8364.1253	-4.8	-0.0403
8364.1573	153663				
8393.0973	8916				
8404.0973	70510				
8421.1170	411115	1-40x1-40, b38	8421.1467	-3.5	-0.0297
8421.2573	411079				
8504.1773	7732				
8519.1273	38215	1-40x1-40, b39	8520.2150	-127.7	-1.0877
8628.2773	7526				

Peak list for Suppl. Fig. 12 Aβ1-38×1-40/Aβ1-40×1-38; $-H_2O$ link Scan 1528 Charge 5+ m/z 1688.6360 RT 10.44 min					
Experimental $[M+H]^+$ [Da]	Intensity	Fragment label	Theoretical $[M+H]^+$ [Da]	Δm [ppm]	Δm [Da]
401.2171	5790				
413.2219	639				
415.2374	2077				
416.2326	1177				
426.2703	664				
430.2506	744				
430.2658	6717				
430.2658	6717				
430.2660	6717	1-40, y05	430.2666	-1.4	-0.0006
431.2703	105				
444.2272	6125				
458.2440	2527				
479.2128	887				
486.3114	1730				
514.3073	3666				
515.2658	3646				
525.3412	1576				
533.2755	4211				
533.2755	4994	1-38, y06	533.2757	-0.5	-0.0003
533.2756	4591				
534.2788	613				
553.7343	599				
557.3123	1177				
561.3064	10011	1-40, y06	561.3070	-1.1	-0.0006
561.3064	6812				
561.3068	9532				
562.3108	894				
563.3489	628				
586.3383	2033				
596.3228	1506				
600.3558	1142				
610.3395	609				

614.3325	9609				
614.3325	7020				
614.3326	9669				
615.3361	475				
619.2844	2534	1-38/40, b05	619.2840	0.6	0.0004
627.3906	1123				
646.3590	12878				
646.3590	8007				
646.3590	13247	1-38, y07	646.3598	-1.2	-0.0008
653.4346	765				
656.3792	1963				
674.3923	1198	1-40, y07	674.3911	1.8	0.0012
675.3005	716				
675.3953	763				
698.4290	701				
708.3849	663				
710.3289	652				
714.6954	711				
727.4160	3113				
731.4122	4249				
731.4122	6683	1-40, y08	731.4126	-0.5	-0.0003
731.4125	6346				
741.4293	1480				
741.7897	888				
742.4932	647				
745.4266	906				
755.4489	2819				
756.3437	5565	1-38/40, b06	756.3429	1.0	0.0008
758.8362	439				
759.4434	3248	1-38, y08	759.4439	-0.6	-0.0005
767.4783	966				
772.3314	6645				
773.3347	103				
784.4755	708				
811.8875	722				
813.4761	904				
840.4952	2681				
841.5027	152				
844.4952	12697	1-40, y09	844.4966	-1.6	-0.0014
871.3684	48523	1-38/40, b07	871.3698	-1.7	-0.0014
871.3687	47621				

872.3721	8086				
872.3722	778				
880.4530	880				
883.5413	969				
890.4994	796				
898.5183	854				
905.3911	5567				
905.8917	819				
911.5320	1719				
939.4107	639				
940.5630	962				
968.5626	1015				
968.9356	4031				
968.9358	4618				
969.9402	1288				
970.9451	23				
997.5917	1041				
1010.6019	2150				
1010.6022	2110				
1011.6056	416				
1015.5958	1751	1-38/40, b09; 1-38, y11	1015.5974	-1.6	-0.0016
1016.6011	435				
1025.9810	1342				
1026.4841	4027				
1066.5066	1169				
1071.8738	1515				
1075.0181	189				
1085.6399	1019	1-40, y12	1085.6393	0.6	0.0006
1099.4695	769				
1099.5371	877				
1129.6380	804	1-38, y12	1129.6403	-2.1	-0.0023
1133.8234	948				
1141.6411	5408				
1141.6411	5723				
1165.0679	1002				
1169.9456	737				
1213.7350	857	1-40, y13	1213.7342	0.6	0.0008
1214.5728	865				
1215.7361	1351				
1216.6713	2410	1-38, y13	1216.6724	-0.9	-0.0011
1216.6727	2156				

1217.6758	529				
1222.5860	4070				
1223.0903	909				
1240.7091	3078				
1241.7131	30				
1243.7102	727				
1259.8635	837				
1262.6282	1030				
1262.9663	2041				
1263.5956	966				
1267.6307	788				
1272.6404	873				
1273.6957	12103	1-38, y14	1273.6938	1.5	0.0019
1274.6985	5948				
1275.7009	1144				
1279.5317	1114				
1281.3057	694				
1291.5729	1163				
1294.7018	169				
1295.6526	3680				
1297.7300	2123				
1307.5287	21727				
1307.5288	22631	1-38/40, b11	1307.5293	-0.4	-0.0005
1328.7782	1910				
1329.9877	1091				
1331.1274	1120				
1333.6682	1370				
1339.3330	8938				
1339.3340	7168				
1349.0671	823				
1351.8815	857				
1354.7470	2419				
1354.7533	2915				
1356.3894	1131				
1372.7614	34727	1-38, y15	1372.7622	-0.6	-0.0009
1372.7616	31364				
1405.0493	5356				
1405.0496	8005				
1405.7086	2038				
1406.5923	15546	1-38/40, b12	1406.5977	-3.8	-0.0054
1412.2570	1455				

1412.3530	1429				
1415.4218	1882				
1416.1765	2141				
1464.7072	1552				
1471.8303	12456				
1471.8307	13479	1-40, y16	1471.8307	0.0	0.0000
1474.7167	2937				
1476.0653	3779				
1476.3878	5780				
1487.7910	3542	1-38, y16	1487.7892	1.2	0.0018
1513.7257	6466				
1515.6616	2748				
1532.7489	4152				
1537.9562	6258				
1543.1558	3881				
1543.6572	33352				
1543.6576	37501	1-38/40, b13	1543.6566	0.7	0.0010
1544.7578	6167				
1548.9703	4464				
1550.7612	11771				
1557.7584	6587				
1559.1721	5418				
1559.7622	10444				
1561.3635	4237				
1562.5076	10120				
1563.7614	6013				
1570.9015	31802	1-40, y17	1570.8991	1.5	0.0024
1571.7810	9794				
1573.5662	7465				
1573.7773	7756				
1578.7808	10389				
1578.9757	3928				
1587.7841	11318				
1588.9948	6570				
1589.3801	7561				
1593.7722	5346				
1594.3927	19617				
1596.7817	21945				
1597.5924	5072				
1604.8001	8959				
1607.1859	5645				

1608.0055	7144				
1608.5968	7771				
1613.4045	5228				
1618.6096	14340				
1625.3888	6094				
1625.6084	9734				
1626.0116	14482				
1631.6044	10252				
1631.8084	11628				
1636.4150	9621				
1636.8146	7763				
1638.0134	8446				
1641.4128	6090				
1652.7195	5070				
1652.7208	1599				
1652.7208	1970				
1653.0559	6728				
1654.2219	6880				
1654.8217	7047				
1658.2267	8553				
1660.8195	12843				
1664.6289	14754				
1676.2490	6705				
1676.8430	12663				
1677.0343	11644				
1680.7125	6824				
1680.7125	3429				
1680.7125	12101	1-38/40, b14	1680.7155	-1.8	-0.0030
1681.7156	2919				
1682.8208	10032				
1685.8298	54697				
1690.6394	75159				
1698.7526	1273				
1739.8369	12830				
1743.5923	8389				
1792.8643	8760				
1806.8816	9497				
1807.6244	7806				
1808.1110	10271				
1808.7656	6510				
1808.7656	3310				

1808.7714	12014	1-38/40, b15	1808.7741	-1.5	-0.0027
1838.8734	5781				
1839.8744	11911				
1866.9286	10624				
1899.1708	8557				
1936.8638	18665	1-38/40, b16	1936.8690	-2.7	-0.0052
1936.8638	10605				
1936.8638	4257				
1937.9564	9241				
1944.4387	6603				
1949.9508	13597				
1973.4645	11328				
1983.0034	7996				
2008.0088	10784				
2020.5075	10496				
2031.9441	6762				
2081.0590	1557	1-38, y21	2081.0741	-7.3	-0.0151
2106.5444	169				
2113.3360	2361				
2113.5186	6590				
2115.0227	843				
2130.7498	2981				
2149.0137	11402	1-38/40, b18	2149.0215	-3.6	-0.0078
2149.0289	5778				
2149.0289	2369				
2167.7720	3412				
2169.1084	2277				
2194.1702	2217	1-38, y22	2194.1582	5.5	0.0120
2211.1280	5659				
2211.4814	3244				
2211.8022	2583				
2212.1064	4014				
2214.0918	373				
2214.5864	2691				
2215.0686	1900				
2254.8213	3019				
2280.1304	2518				
2290.1133	3155				
2290.7656	1407				
2291.0990	2585				
2296.0874	1967	1-38/40, b19	2296.0899	-1.1	-0.0025

2299.8503	2084				
2300.1787	6503				
2300.5037	4124				
2356.4760	2782				
2491.1995	1270				
2492.6836	1291				
2588.3920	1322				
3259.6573	8950	1-38, y31	3259.6574	0.0	-0.0001
3477.1960	17434				
3613.7249	11465				
3677.2585	8324				
3732.7947	10629				
3784.8909	16053				
3787.8585	5505				
3882.9036	16358				
3955.9402	13033				
4014.9834	11149	1-38, y37	4014.9925	-2.3	-0.0091
4014.9909	4948				
4038.9900	35708				
4039.4834	23338				
4054.9840	17248				
4056.4788	8583				
4104.5060	15061				
4105.0205	27565				
4113.0254	7611				
4213.0670	3842	1-40, y39	4213.1293	-14.8	-0.0623
4214.1260	3164				
4215.1390	3916				
4227.0156	5978	1-38x1-40, b01	4227.0358	-4.8	-0.0202
4228.0303	23299				
4228.0303	14966				
4425.1772	24162	1-40x1-38, b01	4425.1726	1.0	0.0046
4425.2105	22430				
5180.4907	33198	1-40x1-38, b07	5180.5077	-3.3	-0.0170
5180.5052	19253				
5919.7890	2964	1-38x1-40, b15	5919.7751	2.3	0.0139
6261.0072	8529	1-38x1-40, b18	6260.022555	157.3	0.9846
6290.1343	4401				
6391.2020	4078				
6604.2176	9034	1-40x1-38, b19	6605.2276	-152.9	-1.0101
6622.1784	4137				

6758.4670	4980					
6869.2410	28661	1-38x1-40, b23	6869.2660	-3.6	-0.0250
6869.2556	23304				
6952.3465	13104	1-40x1-38, b22	6952.3759	-4.2	-0.0294
6968.3172	10084	1-38x1-40, b24	6968.3344	-2.5	-0.0172
6970.3237	10016				
7067.3814	26423				
7067.3930	38284	1-40x1-38, b23	7067.4029	-1.4	-0.0099
7166.4560	11643	1-40x1-38, b24	7166.4713	-2.1	-0.0152
7167.4470	13983				
7482.5684	5908	1-38x1-40, b30	7482.5844	-2.1	-0.0160
7482.5991	5265				
7567.6940	9554				
7578.6665	6512				
7595.6734	18794	1-38x1-40, b31	7595.6685	0.6	0.0049
7596.6680	20874				
7680.7594	7872	1-40x1-38, b30	7680.7212	5.0	0.0382
7690.7470	6928				
7707.7440	4121				
7708.7374	29353				
7708.7393	34743	1-38x1-40, b32	7708.7525	-1.7	-0.0132
7793.8100	21395				
7793.8717	23867	1-40x1-38, b31	7793.8053	8.5	0.0664
7878.8296	38252				
7878.8485	55769	1-38x1-40, b34	7878.8581	-1.2	-0.0096
7878.8500	28990				
7905.8680	9810				
7906.8547	33826	1-40x1-38, b32	7906.8894	-4.4	-0.0347
7906.8877	17217				
7908.8760	10201				
7962.8960	11936	1-40x1-38, b33	7963.9107	-127.4	-1.0147
7992.8973	10684				
8009.8926	69034	1-38x1-40, b35	8009.8985	-0.7	-0.0059
8009.9174	40548				
8010.8825	15360				
8062.9936	5311				
8076.9676	69030	1-40x1-38, b34	8076.9949	-3.4	-0.0273
8076.9746	56331				
8092.9637	15701				
8108.9891	53611	1-38x1-40, b36	8108.9670	2.7	0.0221
8109.9556	53903				

8109.9579	7282				
8132.0331	6704				
8148.0134	5692				
8165.9880	27739	1-38x1-40, b37	8165.9884	-0.1	-0.0004
8191.0130	24590				
8207.9747	104812	1-40x1-38, b35	8208.0354	-7.4	-0.0607
8208.0250	102614				
8221.9950	8830				
8223.0114	78681	1-38x1-40, b38	8223.0099	0.2	0.0015
8279.0312	7281				
8293.0900	28169				
8307.0900	120935	1-40x1-38, b36	8307.1038	-1.7	-0.0138
8307.1123	110903				
8322.0660	126000	1-38x1-40, b39	8322.0783	-1.5	-0.0123
8323.0815	117138				
8364.0764	37206	1-40x1-38, b37	8364.1253	-5.8	-0.0489
8403.1077	9845				
8422.1177	70423				
8423.1090	45286				
8439.1480	464355	1-38x1-40 M	8439.1567	-1.0	-0.0087
8439.2204	464333				

Peak list for Suppl. Fig. 13 Aβ1-42×1-42; -H_2O link; -NH_3 link; merged scans Scans 1625-1654 Charge 6+ Selected m/z 1502.76 RT 9.83-9.98 min								
Experimental $[M+H]^+$ [Da]	Intensity	Fragment label	Theoretical $[M+H]^+$; -H_2O link [Da]	Δm; -H_2O link [ppm]	Δm; -H_2O link [Da]	Theoretical $[M+H]^+$; -NH_3 link [Da]	Δm; -NH_3 link [ppm]	Δm; -NH_3 link [Da]
401.22168	217							
409.20697	368							
412.2556	733							
416.2328	210							
426.27118	2564							
427.21753	294							
443.19147	75							
444.22766	310							
461.20203	175							
475.21613	75							
497.3449	52							
501.2541	111							
514.3059	89							
515.2644	241							
515.31934	260	y06	515.3193	0.0	0.0000	515.3193	0.0	0.0000
517.2279	267							
525.33997	307							
535.23926	77							
539.27075	83							
543.29626	404							
557.3113	77							
591.2639	62							
614.3328	1085							
614.387	672	y07	614.3877	-1.2	-0.0007	614.3877	-1.2	-0.0007
653.43536	54							
654.2213	54							
656.3805	242							
699.4219	88							
703.8002	80							
713.40076	1189							

727.41547	472							
745.427	422	y08	745.4282	-1.6	-0.0012	745.4282	-1.6	-0.0012
756.3423	533	b06	756.3429	-0.8	-0.0006	756.3429	-0.8	-0.0006
766.03436	54							
771.9649	84							
815.3909	93							
826.48474	1195							
833.39386	56							
839.40405	75							
840.49805	58							
856.84607	78							
871.3688	2234	b07	871.3698	-1.2	-0.0010	871.3698	-1.2	-0.0010
882.08435	65							
882.7511	57							
888.4072	84							
911.529	65							
915.5321	476	y10	915.5337	-1.8	-0.0016	915.5337	-1.8	-0.0016
921.0947	96							
933.4306	66							
939.567	256							
952.4466	67							
974.16724	107							
974.23474	136							
997.5139	159							
1027.3125	66							
1028.6177	367	y11	1028.6178	-0.1	-0.0001	1028.6178	-0.1	-0.0001
1034.1428	71							
1055.9563	65							
1075.5112	219							
1104.3081	87							
1106.9136	77							
1119.5195	117							
1152.0371	81							
1153.2174	73							
1162.9305	92							
1189.7122	81							
1206.5905	130							

1211.9854	101							
1213.5125	150							
1218.6011	98							
1226.5642	118							
1235.7628	104							
1236.198	129							
1250.6106	108							
1257.0754	168							
1258.6068	162							
1259.3892	176							
1294.6296	156							
1325.8209	363							
1403.686	769							
1451.7029	675							
1452.0903	668							
1467.9022	453							
1468.9053	875							
1575.1719	615							
1596.182	966							
1597.185	1088							
1620.6035	1702							
1650.6184	931							
1653.4207	650							
1653.625	1512							
1653.8254	3732							
1699.834	1409							
1700.0488	879							
1700.4502	1529							
1741.4636	569							
1742.4667	1020							
1762.283	304							
1762.677	394							
1787.8678	197							
1790.8718	421							
1792.8665	147							
1808.7681	260							
1816.1619	115							
1831.3688	116							
1832.3859	120							
1833.8851	299							
1835.1454	110							

1835.9851	140							
1841.1774	129							
1849.1334	141							
1849.4769	111							
1857.8912	163							
1873.1888	144							
1875.6315	119							
1886.9094	104							
1889.4128	209							
1899.1627	120							
1905.1677	237							
1906.903	136							
1913.9128	135							
1936.8646	194							
1940.9681	154							
1947.8514	150							
1952.4751	141							
1958.7046	118							
1991.2263	341							
1991.46	220							
1995.9694	171							
2019.4701	123							
2023.9938	125							
2025.9855	253							
2029.1266	174							
2038.4904	140							
2049.0012	75							
2049.9868	257							
2051.0098	65							
2052.4963	114							
2053.2532	69							
2060.167	96							
2063.7017	65							
2065.7705	70							
2073.2822	67							
2073.7537	1							
2092.254	166							
2097.033	64							
2097.2666	213							
2099.037	79							
2099.2747	83							

2100.0173	67							
2104.3875	58							
2111.9883	73							
2121.789	155							
2163.3833	63							
2176.0708	58							
2227.2056	111							
2247.1042	63							
2256.1223	192							
2257.1436	2							
2259.0044	62							
2260.149	89							
2274.2932	72							
2296.0808	214							
2305.1396	69							
2346.417	61							
2357.896	156							
2424.9673	57							
2443.1792	75							
2457.515	69							
2460.1426	117							
2474.6914	66							
2556.4756	56							
2568.598	323							
2582.2405	354							
2629.1218	66							
2630.6675	62							
2691.9014	98							
2697.314	862							
2698.659	628							
2768.162	62							
2780.3525	188							
2790.4434	55							
2831.7256	1030							
2839.1997	64							
2857.331	309							
2914.341	180							
2957.4478	2186							
3005.1528	3848							
3005.8228	1508							
3892.8787	217							

3996.938	759							
4197.0693	3686							
4197.556	2156							
4501.2114	2754							
4506.2495	2218							
4512.2705	289							
7864.806	1873	1-42x1-42, b30	7864.8424	-4.6	-0.0364	7865.8264	-129.7	-1.0204
7980.8984	3637							
8090.9766	5300	1-42x1-42, b32	8091.0105	-4.2	-0.0339	8091.9946	-125.8	-1.0180
8096.963	2001							
8149.003	3664	1-42x1-42, b33	8148.0319	119.2	0.9711	8149.0159	-1.6	-0.0129
8149.9893	3882							
8262.084	9441	1-42x1-42, b34	8261.1159	117.2	0.9681	8262.1000	-1.9	-0.0160
8263.079	9125							
8292.024	159							
8393.121	14231	1-42x1-42, b35	8392.1564	114.9	0.9646	8393.1405	-2.3	-0.0195
8550.216	2516	1-42x1-42, b37	8548.2460	230.4	1.9700	8549.2300	115.3	0.9860
8606.222	4916							
8607.237	9867	1-42x1-42, b38	8605.2674	228.8	1.9696	8606.2515	114.5	0.9855
8705.296	3128	1-42x1-42, b39	8704.3362	110.3	0.9598	8705.3202	-2.8	-0.0242
8706.292	1727							
8995.456	2283							
9006.492	13212	1-42x1-42 M	9005.5358	106.2	0.9562	9006.5198	-3.1	-0.0278

Peak list for Suppl. Fig. 14
Aβ1-42×1-42; DiY-link
Scan 2184
Charge 6+
m/z 1504.4309
RT 10.75 min

Experimental $[M+H]^+$ [Da]	Intensity	Fragment label	Theoretical $[M+H]^+$ [Da]	Δm [ppm]	Δm [Da]
401.2170	8049				
401.2740	24738				
401.2741	25652				
401.2741	23037				
410.3726	949				
412.2536	52805				
412.2538	53061				
412.2538	45226				
416.2300	14300				
426.2691	126794				
426.2691	164579				
426.2692	164579				
427.2729	11879				
427.2730	4944				
430.2467	1075				
444.2257	19183				
444.2257	23851				
444.2258	23327				
445.5736	906				
450.4605	1092				
458.2408	6747				
458.2953	31503				
458.2954	32034				
458.9346	1005				
461.0951	1308				
467.2947	891				
469.3104	1712				
497.3058	8508				
497.3426	3474				
498.3466	750				
514.3035	2817				
515.0082	1650				

515.2632	17607				
515.2634	12591				
515.2634	17970				
515.3167	240888				
515.3168	142782				
515.3168	242666				
515.6317	1173				
516.2655	340				
518.3237	1337				
523.2971	1031				
525.3375	37064				
525.3375	23937				
525.3375	36595				
526.3417	94				
543.2937	40419				
543.2937	25754				
543.2937	40915				
544.2966	365				
555.5493	1125				
557.3093	8948				
571.3247	1956				
574.9724	1153				
586.3355	12981				
586.3355	21805				
586.3357	21630				
587.3391	285				
596.3187	3985				
596.3744	3593				
614.3306	36592				
614.3306	19775				
614.3307	36567				
614.3846	148828				
614.3846	70354				
614.3846	149238				
615.3878	180				
628.3447	12714				
628.3831	3816				
656.3765	17727				
656.3765	37603				
656.3768	37202				
657.3804	1837				

673.7047	1225				
673.7374	1087				
685.4038	3506				
686.4077	462				
695.3854	1117				
696.1725	1182				
699.4192	12751				
699.4192	6263				
699.4193	12021				
700.4222	2017				
713.3980	68534				
714.4025	23193				
714.4025	11483				
715.4015	2407				
722.5981	1112				
727.4138	29977				
727.4138	13847				
727.4140	30628				
728.4155	617				
741.4279	4173				
745.4244	157522				
745.4244	153408				
747.4256	11202				
747.4257	1030				
756.3377	3013				
756.9504	1392				
769.4607	6254				
769.4608	6524				
769.4608	3860				
770.4631	135				
776.9428	2020				
777.9493	715				
784.4708	1213				
798.4858	6697				
799.9646	1870				
809.4765	1138				
812.4679	1341				
816.5106	1622				
826.4815	87574				
826.4818	91200				
828.4854	3171				

833.4846	1894				
840.4970	9561				
840.4971	9281				
840.4971	5189				
858.5076	8069				
858.5076	21312				
858.5078	20911				
859.5104	2032				
871.3655	97929				
871.3655	95333				
873.3693	4698				
874.3699	769				
878.5123	1762				
897.5171	1214				
911.5286	2151				
915.5289	201153				
915.5291	200931				
916.5316	4620				
916.5319	31032				
939.4893	1329				
939.5650	40204				
939.5654	40231				
940.5640	419				
940.5679	6365				
941.5670	199				
942.5682	918				
968.5551	7615				
994.0363	1421				
996.4859	1153				
997.5826	1358				
1002.2073	3827				
1002.5411	1862				
1010.5982	2949				
1028.6123	140563				
1028.6126	147845				
1029.6150	9218				
1031.6196	1168				
1052.6484	6730				
1052.6486	7100				
1053.6509	384				
1067.6233	7545				

1082.6292	1374				
1090.5600	1520				
1141.6355	3337				
1141.6929	46609				
1141.6931	47450				
1142.0032	1691				
1142.6982	2052				
1143.6985	234				
1180.7065	3263				
1184.5400	1793				
1198.6540	1698				
1255.6759	7952				
1256.6650	1808				
1259.7723	1680				
1260.1959	1630				
1269.7534	22788				
1269.7575	26965				
1270.7565	5692				
1271.6222	2801				
1313.9716	8211				
1347.3319	11913				
1349.1544	8214				
1354.7444	9727				
1373.6716	10076				
1380.5200	7557				
1381.1846	7029				
1383.8471	17535				
1392.5121	8175				
1394.1773	10545				
1394.6716	17832				
1399.8595	12405				
1400.6930	11923				
1402.5214	17423				
1403.3638	33286				
1405.8588	27602				
1406.3489	13940				
1406.6857	8405				
1410.5328	7987				
1411.3680	9421				
1412.5298	12114				
1414.6798	15987				

1425.3676	11473				
1427.5400	18343				
1430.0392	14051				
1433.8702	22850				
1441.3904	11807				
1444.0535	22377				
1444.3822	11198				
1445.7164	16803				
1452.7205	23291				
1457.8914	20336				
1458.2273	27005				
1458.4003	12672				
1458.5513	12005				
1467.3931	27682				
1468.2313	51568				
1469.5656	17266				
1469.7229	15228				
1473.7206	14558				
1473.9022	15044				
1477.1067	11422				
1477.9139	13534				
1479.5808	12591				
1487.0818	11628				
1494.7384	12436				
1502.0862	41298				
1506.0851	11811				
1508.3370	10980				
1511.3337	11479				
1516.5348	7867				
1517.7240	7956				
1518.1368	9360				
1520.3339	14421				
1523.3346	7668				
1529.3169	7294				
1534.1465	31743				
1553.7576	59473				
1555.3589	13832				
1555.9973	13937				
1557.5667	9011				
1560.5531	13901				
1567.7694	16201				

1568.3672	8528				
1570.9696	11313				
1571.1722	15722				
1574.1679	17733				
1575.3748	13436				
1579.1646	10531				
1579.7721	11529				
1601.9977	15914				
1613.5931	18714				
1619.9890	14394				
1624.7809	19472				
1628.0114	11429				
1628.3821	8420				
1632.7709	17155				
1647.6150	14156				
1647.8273	24512				
1648.0099	8673				
1648.2202	31461				
1649.4010	15214				
1650.6108	9013				
1655.9636	8468				
1656.9442	7635				
1660.4137	11475				
1660.6165	14156				
1660.8153	17295				
1661.2150	13926				
1668.4347	9390				
1668.6117	13390				
1675.2300	16755				
1680.8287	27237				
1687.4315	10896				
1689.0466	18661				
1689.8013	13713				
1692.8197	13868				
1694.2573	11042				
1697.2388	13497				
1739.0557	31501				
1743.0668	31623				
1759.4811	14151				
1818.3806	12961				
1841.6383	18566				

1842.1449	48028				
1842.6276	14119				
1845.6322	20257				
1856.1387	15685				
1873.9125	15600				
1900.1722	19430				
1939.2183	12978				
1941.9496	15102				
1970.7144	20781				
1972.2129	15779				
1998.7355	24269				
2103.7918	14114				
2129.7940	10301				
2131.0444	27114				
2131.3052	11345				
2155.8113	33088				
2156.3150	21295				
2156.8145	9779				
2570.2470	4471				
2588.5928	13670				
2968.1419	9727				
3682.7803	48962				
3882.3865	55582				
3895.8872	59099				
3896.3810	70410				
3903.3810	36200				
3939.4200	46620				
3939.9048	58718				
3939.9266	41905				
4094.0240	6067				
4132.5420	13313				
4184.5557	4263				
4193.5512	5169				
4196.0504	15888				
4204.0469	22150				
4209.0596	34534				
4223.5821	6089				
4310.1190	36580				
4323.6399	8106				
4344.1406	9445				
4382.2042	6910				

4385.6799	11283				
4394.6691	14422				
4396.1710	10910				
4425.6945	7906				
4455.2161	4108				
7192.4456	9837	αb32+βb32	7192.4800	-4.8	-0.0344
7249.4550	30001	αb34+βb31; αb31+βb34; αb33+βb32; αb32+βb33	7249.5014	-6.4	-0.0464
7250.4697	15467				
7267.4728	19954				
7267.4795	30001	αb30+βb35; αb35+βb30; αb23+βb42	7267.5189	-5.4	-0.0394
7363.5148	27685	αb34+βb32; αb32+βb34	7362.5854	126.2	0.9294
7367.5393	9243				
7421.4042	16133				
7479.5513	20582				
7479.5714	34950	αb31+βb36; αb36+βb31	7479.6103	-5.2	-0.0390
7493.6241	24310				
7494.5845	24514	αb32+βb35; αb35+βb32	7494.5864	-0.3	-0.0019
7532.6242	15007	αb34+βb34	7532.6910	-8.9	-0.0668
7533.6237	13985				
7550.6141	21673	αb33+βb35; αb35+βb33	7550.6475	-4.4	-0.0333
7578.6448	13806				
7592.6510	41431	αb32+βb36; αb36+βb32	7592.6944	-5.7	-0.0434
7592.6530	33774				
7648.6933	16256				
7649.6774	18088	αb33+βb36; αb36+βb33; αb32+βb37; αb37+βb32	7649.7159	-5.0	-0.0385
7663.7260	64601	αb34+βb35; αb28+βb41; αb35+βb34	7663.7315	-0.7	-0.0055
7664.6997	25215				
7677.6921	20448				
7691.7399	53057	αb31+βb39; αb39+βb31	7692.7215	-127.6	-0.9816
7706.7002	46373	αb33+βb37; αb37+βb33; αb32+βb38; αb38+βb32	7706.7373	-4.8	-0.0371
7762.7676	25839	αb34+βb36; αb36+βb34; αb33+βb38; αb38+βb33	7762.7999	-4.2	-0.0324
7778.7193	13126				
7791.8199	115069	αb31+βb40; αb30+βb41; αb41+βb30; αb40+βb31	7791.7901	3.8	0.0298
7805.7745	84143	αb32+βb39; αb39+βb32	7805.8057	-4.0	-0.0313
7819.7736	17517	αb34+βb37; αb37+βb34	7819.8214	-6.1	-0.0478
7861.8064	35448	αb33+βb39; αb39+βb33	7862.8271	-129.8	-1.0207
7876.7821	71799	αb34+βb38; αb38+βb34	7876.8429	-7.7	-0.0608

7881.8072	20473	αb30+βb42; αb42+βb30	7880.8371	123.1	0.9701
7893.8561	38889	αb36+βb35; αb35+βb36	7893.8404	2.0	0.0157
7904.8051	150364				
7904.8247	227805	αb31+βb41; αb41+βb31; αb32+βb40; αb40+βb32	7904.8742	-6.3	-0.0495
7948.8945	40249				
7961.7790	35080	αb33+βb40; αb40+βb33	7961.8956	-14.6	-0.1166
7975.8613	162645	αb34+βb39; αb39+βb34	7975.9113	-6.3	-0.0500
7975.9385	110197				
7993.8725	122622	αb36+βb36; αb31+βb42; αb42+βb31	7993.9213	-6.1	-0.0488
7993.8870	43444				
8007.8406	65101	αb38+βb35; αb35+βb38	8007.8833	-5.3	-0.0427
8017.9162	39929	αb32+βb41; αb41+βb32	8017.9582	-5.2	-0.0421
8045.9411	11569				
8051.9401	15608				
8058.9146	11640				
8074.9193	162653	αb34+βb40; αb33+βb41; αb41+βb33; αb40+βb34	8074.9797	-7.5	-0.0604
8074.9536	35980				
8075.9381	13554				
8106.9126	44135				
8106.9237	340364				
8106.9340	463168	αb39+βb35; αb35+βb39; αb38+βb36; αb36+βb38; αb37+βb37; αb32+βb42; αb42+βb32	8107.0054	-8.8	-0.0714
8163.9973	105697	αb38+βb37; αb37+βb38; αb33+βb42; αb42+βb33	8164.0268	-3.6	-0.0295
8176.9796	37287				
8188.0070	82613	αb34+βb41; αb41+βb34	8188.0637	-6.9	-0.0567
8205.9780	351217	αb39+βb36; αb36+βb39; αb40+βb35; αb35+βb40	8206.0202	-5.1	-0.0422
8206.0010	51540				
8206.0551	280925				
8220.9526	51466	αb38+βb38	8220.9947	-5.1	-0.0421
8262.9849	87251	αb39+βb37; αb37+βb39	8263.0416	-6.9	-0.0568
8276.0444	20769				
8276.0880	30012				
8277.0750	257950	αb34+βb42; αb42+βb34	8277.1109	-4.3	-0.0359
8277.1129	210938				
8281.0794	4183				
8291.0893	48281				
8305.0450	23492				
8305.0957	193177	αb40+βb36; αb36+βb40	8305.0886	0.9	0.0071

8319.9541	299219	αb39+βb38; αb38+βb39	8320.0631	-13.1	-0.1090
8320.0440	272518				
8362.0903	105029	αb40+βb37; αb37+βb40	8362.1101	-2.4	-0.0197
8382.0823	11251				
8391.1010	116995				
8402.1296	15120				
8407.1320	17588				
8408.0791	223158	αb42+βb35; αb35+βb42	8408.1514	-8.6	-0.0723
8419.1090	837244	αb39+βb39; αb40+βb38; αb38+βb40	8419.1315	-2.7	-0.0225
8419.1518	630283				
8475.1487	62374	αb41+βb37; αb37+βb41	8475.1941	-5.4	-0.0454
8490.1628	177299				
8502.1664	17570				
8507.1840	287684				
8507.1989	349318	αb42+βb36; αb36+βb42	8507.2198	-2.5	-0.0209
8517.1660	308703				
8518.1540	495053				
8518.1950	13885				
8518.2338	655781	αb40+βb39; αb39+βb40	8518.1999	4.0	0.0339
8532.1477	172298	αb41+βb38; αb38+βb41	8532.2156	-8.0	-0.0679
8564.1979	138378	αb42+βb37; αb37+βb42	8564.2413	-5.1	-0.0434
8574.1844	11556				
8588.2077	36719				
8597.2606	6446				
8603.2198	152359				
8616.3000	166210				
8618.2160	511172	αb40+βb40	8617.2682	110.0	0.9478
8618.2332	21797				
8620.2180	545079				
8620.2495	821346	αb42+βb38; αb38+βb42	8621.2626	-117.5	-1.0131
8631.2187	372113	αb41+βb39; αb39+βb41	8631.2840	-7.6	-0.0652
8677.2954	37176				
8692.3408	132894				
8703.3361	120877				
8720.2890	1363990	αb42+βb39; αb39+βb42	8720.3311	-4.8	-0.0421
8720.3270	3739				
8720.3302	1239131				
8730.2990	560277				
8730.2996	579556	αb41+βb40; αb40+βb41	8730.3524	-6.0	-0.0528
8761.3269	10176				
8776.4089	30611				

8792.3363	9569				
8803.3372	100866				
8819.3550	1701501	αb42+βb40; αb40+βb42	8819.3995	-5.1	-0.0445
8819.3779	1635989				
8830.3599	11883				
8843.3186	127293	αb41+βb41	8843.4365	-13.3	-0.1179
8886.3888	10179				
8891.3795	9048				
8915.3999	42004				
8921.3953	6176				
8932.4280	624615	αb42+βb41; αb41+βb42	8932.4836	-6.2	-0.0556
8932.5217	624548				
9003.4534	50722				
9021.4839	69428	αb42+βb42	9021.5307	-5.2	-0.0469
Experimental $[M+H]^+$ [Da]	Intensity	Fragment label	Theoretical $[M+H]^+$ [Da]	Δm [ppm]	Δm [Da]

Supplementary Table 4

Amyloid-β17-28×1-5, –H_2O link, b-, y-fragments			
Sequence (α+β)	Label style 1	Label style 2	Deconvoluted mass [M+H]+
G	α9-9	αi9	58.02929
A	α5-5	αi5	72.04494
A	β2-2	βi2	72.04494
S	α10-10	αi10	88.03985
V	α8-8	αi8	100.07624
V	α2-2	αi2	100.07624
E	α6-6	αi6	112.03985
<L	α1-1	αb1	114.09189
N	α11-11	αi11	115.05075
D	β1-1	βb1	116.03477
D	α7-7	αi7	116.03477
E	β3-3	βi3	130.05042
GS	α9-10	αi9-10	145.06132
K>	α12-12	αy1	147.11335
F	α3-3	αi3	148.07624
F	α4-4	αi4	148.07624
F	β4-4	βi4	148.07624
VG	α8-9	αi8-9	157.0977
R>	β5-5	βy1	175.1195
AE	α5-6	αi5-6	183.07697
DA	β1-2	βb2	187.07188
AE	β2-3	βi2-3	201.08753
SN	α10-11	αi10-11	202.08278
<LV	α1-2	αb2	213.1603
DV	α7-8	αi7-8	215.10318
FA	α4-5	αi4-5	219.11335
E+D	α6-6+β1-1	αi6+βb1	227.0668
ED	α6-7	αi6-7	227.0668
VGS	α8-10	αi8-10	244.12973
VF	α2-3	αi2-3	247.14465
GSN	α9-11	αi9-11	259.10424
NK>	α11-12	αy2	261.15628
DVG	α7-9	αi7-9	272.12465
EF	β3-4	βi3-4	277.11883
FF	α3-4	αi3-4	295.14465

E+DA	α6-6+β1-2	αi6+βb2	298.10391
AE+D	α5-6+β1-1	αi5-6+βb1	298.10391
AED	α5-7	αi5-7	298.10391
DAE	β1-3	βb3	316.11447
FR>	β4-5	βγ2	322.18791
EDV	α6-8	αi6-8	326.13521
FAE	α4-6	αi4-6	330.14538
ED+D	α6-7+β1-1	αi6-7+βb1	342.09374
AEF	β2-4	βi2-4	348.15595
SNK>	α10-12	αγ3	348.18831
VGSN	α8-11	αi8-11	358.17266
DVGS	α7-10	αi7-10	359.15667
<LVF	α1-3	αb3	360.22872
FFA	α3-5	αi3-5	366.18177
AE+DA	α5-6+β1-2	αi5-6+βb2	369.14102
EDVG	α6-9	αi6-9	383.15667
VFF	α2-4	αi2-4	394.21307
AEDV	α5-8	αi5-8	397.17232
GSNK>	α9-12	αγ4	405.20977
AED+D	α5-7+β1-1	αi5-7+βb1	413.13085
ED+DA	α6-7+β1-2	αi6-7+βb2	413.13085
E+DAE	α6-6+β1-3	αi6+βb3	427.1465
EDV+D	α6-8+β1-1	αi6-8+βb1	441.16215
FAE+D	α4-6+β1-1	αi4-6+βb1	445.17232
FAED	α4-7	αi4-7	445.17232
EFR>	β3-5	βγ3	451.23051
AEDVG	α5-9	αi5-9	454.19379
DAEF	β1-4	βb4	463.18289
VFFA	α2-5	αi2-5	465.25018
EDVGS	α6-10	αi6-10	470.1887
DVGSN	α7-11	αi7-11	473.1996
FFAE	α3-6	αi3-6	477.21379
AED+DA	α5-7+β1-2	αi5-7+βb2	484.16797
EDVG+D	α6-9+β1-1	αi6-9+βb1	498.18362
AE+DAE	α5-6+β1-3	αi5-6+βb3	498.18362
VGSNK>	α8-12	αγ5	504.27818
<LVFF	α1-4	αb4	507.29713
EDV+DA	α6-8+β1-2	αi6-8+βb2	512.19927
AEDV+D	α5-8+β1-1	αi5-8+βb1	512.19927
FAE+DA	α4-6+β1-2	αi4-6+βb2	516.20944

AEFR>	β2-5	βy4	522.26762
AEDVGS	α5-10	αi5-10	541.22582
ED+DAE	α6-7+β1-3	αi6-7+βb3	542.17345
FAEDV	α4-8	αi4-8	544.24074
FAED+D	α4-7+β1-1	αi4-7+βb1	560.19927
AEDVG+D	α5-9+β1-1	αi5-9+βb1	569.22073
EDVG+DA	α6-9+β1-2	αi6-9+βb2	569.22073
E+DAEF	α6-6+β1-4	αi6+βb4	574.21492
VFFAE	α2-6	αi2-6	576.28221
<LVFFA	α1-5	αb5	578.33424
AEDV+DA	α5-8+β1-2	αi5-8+βb2	583.23638
EDVGSN	α6-11	αi6-11	584.23163
EDVGS+D	α6-10+β1-1	αi6-10+βb1	585.21564
FFAE+D	α3-6+β1-1	αi3-6+βb1	592.24074
FFAED	α3-7	αi3-7	592.24074
FAEDVG	α4-9	αi4-9	601.2622
AED+DAE	α5-7+β1-3	αi5-7+βb3	613.21056
DVGSNK>	α7-12	αy6	619.30513
FAED+DA	α4-7+β1-2	αi4-7+βb2	631.23638
DAEFR>	β1-5	βfull (βy5)	637.29456
AEDVG+DA	α5-9+β1-2	αi5-9+βb2	640.25784
EDV+DAE	α6-8+β1-3	αi6-8+βb3	641.24186
FAE+DAE	α4-6+β1-3	αi4-6+βb3	645.25203
AE+DAEF	α5-6+β1-4	αi5-6+βb4	645.25203
AEDVGSN	α5-11	αi5-11	655.26874
AEDVGS+D	α5-10+β1-1	αi5-10+βb1	656.25276
EDVGS+DA	α6-10+β1-2	αi6-10+βb2	656.25276
FAEDV+D	α4-8+β1-1	αi4-8+βb1	659.26768
FFAE+DA	α3-6+β1-2	αi3-6+βb2	663.27785
FAEDVGS	α4-10	αi4-10	688.29423
ED+DAEF	α6-7+β1-4	αi6-7+βb4	689.24186
<LVFFAE	α1-6	αb6	689.36627
VFFAED	α2-7	αi2-7	691.30915
VFFAE+D	α2-6+β1-1	αi2-6+βb1	691.30915
FFAEDV	α3-8	αi3-8	691.30915
EDVG+DAE	α6-9+β1-3	αi6-9+βb3	698.26332
EDVGSN+D	α6-11+β1-1	αi6-11+βb1	699.25857
FFAED+D	α3-7+β1-1	αi3-7+βb1	707.26768
AEDV+DAE	α5-8+β1-3	αi5-8+βb3	712.27897
FAEDVG+D	α4-9+β1-1	αi4-9+βb1	716.28914

AEDVGS+DA	α5-10+β1-2	αi5-10+βb2	727.28987
FAEDV+DA	α4-8+β1-2	αi4-8+βb2	730.30479
EDVGSNK>	α6-12	αy7	730.33716
E+DAEFR>	α6-6+β1-5	αi6+βfull	748.32659
FFAEDVG	α3-9	αi3-9	748.33061
FAED+DAE	α4-7+β1-3	αi4-7+βb3	760.27897
AED+DAEF	α5-7+β1-4	αi5-7+βb4	760.27897
VFFAE+DA	α2-6+β1-2	αi2-6+βb2	762.34626
AEDVG+DAE	α5-9+β1-3	αi5-9+βb3	769.30044
AEDVGSN+D	α5-11+β1-1	αi5-11+βb1	770.29569
EDVGSN+DA	α6-11+β1-2	αi6-11+βb2	770.29569
FFAED+DA	α3-7+β1-2	αi3-7+βb2	778.30479
EDVGS+DAE	α6-10+β1-3	αi6-10+βb3	785.29535
FAEDVG+DA	α4-9+β1-2	αi4-9+βb2	787.32626
EDV+DAEF	α6-8+β1-4	αi6-8+βb4	788.31027
VFFAEDV	α2-8	αi2-8	790.37756
FAE+DAEF	α4-6+β1-4	αi4-6+βb4	792.32044
FFAE+DAE	α3-6+β1-3	αi3-6+βb3	792.32044
AEDVGSNK>	α5-12	αy8	801.37427
FAEDVGSN	α4-11	αi4-11	802.33716
FAEDVGS+D	α4-10+β1-1	αi4-10+βb1	803.32117
<LVFFAE+D	α1-6+β1-1	αb6+βb1	804.39321
<LVFFAED	α1-7	αb7	804.39321
VFFAED+D	α2-7+β1-1	αi2-7+βb1	806.33609
FFAEDV+D	α3-8+β1-1	αi3-8+βb1	806.33609
AE+DAEFR>	α5-6+β1-5	αi5-6+βfull	819.3637
FFAEDVGS	α3-10	αi3-10	835.36264
AEDVGSN+DA	α5-11+β1-2	αi5-11+βb2	841.3328
EDVG+DAEF	α6-9+β1-4	αi6-9+βb4	845.33174
EDVGSNK>+D	α6-12+β1-1	αy7+βb1	845.3641
VFFAEDVG	α2-9	αi2-9	847.39903
AEDVGS+DAE	α5-10+β1-3	αi5-10+βb3	856.33246
AEDV+DAEF	α5-8+β1-4	αi5-8+βb4	859.34739
FAEDV+DAE	α4-8+β1-3	αi4-8+βb3	859.34739
ED+DAEFR>	α6-7+β1-5	αi6-7+βfull	863.35353
FFAEDVG+D	α3-9+β1-1	αi3-9+βb1	863.35756
FAEDVGS+DA	α4-10+β1-2	αi4-10+βb2	874.35829
<LVFFAE+DA	α1-6+β1-2	αb6+βb2	875.43033
VFFAED+DA	α2-7+β1-2	αi2-7+βb2	877.37321
FFAEDV+DA	α3-8+β1-2	αi3-8+βb2	877.37321

VFFAE+DAE	α2-6+β1-3	αi2-6+βb3	891.38886
EDVGSN+DAE	α6-11+β1-3	αi6-11+βb3	899.33828
<LVFFAEDV	α1-8	αb8	903.46163
VFFAEDV+D	α2-8+β1-1	αi2-8+βb1	905.40451
FAED+DAEF	α4-7+β1-4	αi4-7+βb4	907.34739
FFAED+DAE	α3-7+β1-3	αi3-7+βb3	907.34739
AEDVG+DAEF	α5-9+β1-4	αi5-9+βb4	916.36885
FAEDVG+DAE	α4-9+β1-3	αi4-9+βb3	916.36885
AEDVGSNK>+D	α5-12+β1-1	αy8+βb1	916.40121
EDVGSNK>+DA	α6-12+β1-2	αy7+βb2	916.40121
FAEDVGSN+D	α4-11+β1-1	αi4-11+βb1	917.3641
<LVFFAED+D	α1-7+β1-1	αb7+βb1	919.42016
EDVGS+DAEF	α6-10+β1-4	αi6-10+βb4	932.36376
AED+DAEFR>	α5-7+β1-5	αi5-7+βfull	934.39065
FFAEDVG+DA	α3-9+β1-2	αi3-9+βb2	934.39467
VFFAEDVGS	α2-10	αi2-10	934.43106
FFAE+DAEF	α3-6+β1-4	αi3-6+βb4	939.38886
FAEDVGSNK>	α4-12	αy9	948.44268
FFAEDVGSN	α3-11	αi3-11	949.40557
FFAEDVGS+D	α3-10+β1-1	αi3-10+βb1	950.38959
<LVFFAEDVG	α1-9	αb9	960.48309
EDV+DAEFR>	α6-8+β1-5	αi6-8+βfull	962.42195
VFFAEDVG+D	α2-9+β1-1	αi2-9+βb1	962.42597
FAE+DAEFR>	α4-6+β1-5	αi4-6+βfull	966.43212
AEDVGSN+DAE	α5-11+β1-3	αi5-11+βb3	970.37539
VFFAEDV+DA	α2-8+β1-2	αi2-8+βb2	976.44162
AEDVGSNK>+DA	α5-12+β1-2	αy8+βb2	987.43833
FAEDVGSN+DA	α4-11+β1-2	αi4-11+βb2	988.40121
<LVFFAED+DA	α1-7+β1-2	αb7+βb2	990.45727
AEDVGS+DAEF	α5-10+β1-4	αi5-10+βb4	1003.40088
FAEDVGS+DAE	α4-10+β1-3	αi4-10+βb3	1003.40088
<LVFFAE+DAE	α1-6+β1-3	αb6+βb3	1004.47292
FAEDV+DAEF	α4-8+β1-4	αi4-8+βb4	1006.4158
VFFAED+DAE	α2-7+β1-3	αi2-7+βb3	1006.4158
FFAEDV+DAE	α3-8+β1-3	αi3-8+βb3	1006.4158
<LVFFAEDV+D	α1-8+β1-1	αb8+βb1	1018.48857
EDVG+DAEFR>	α6-9+β1-5	αi6-9+βfull	1019.44341
FFAEDVGS+DA	α3-10+β1-2	αi3-10+βb2	1021.4267
AEDV+DAEFR>	α5-8+β1-5	αi5-8+βfull	1033.45906
VFFAEDVG+DA	α2-9+β1-2	αi2-9+βb2	1033.46308

VFFAE+DAEF	α2-6+β1-4	αi2-6+βb4	1038.45727
EDVGSNK>+DAE	α6-12+β1-3	αy7+βb3	1045.44381
EDVGSN+DAEF	α6-11+β1-4	αi6-11+βb4	1046.40669
<LVFFAEDVGS	α1-10	αb10	1047.51512
VFFAEDVGSN	α2-11	αi2-11	1048.47398
VFFAEDVGS+D	α2-10+β1-1	αi2-10+βb1	1049.458
FFAED+DAEF	α3-7+β1-4	αi3-7+βb4	1054.4158
FFAEDVG+DAE	α3-9+β1-3	αi3-9+βb3	1063.43726
FAEDVG+DAEF	α4-9+β1-4	αi4-9+βb4	1063.43726
FAEDVGSNK>+D	α4-12+β1-1	αy9+βb1	1063.46963
FFAEDVGSN+D	α3-11+β1-1	αi3-11+βb1	1064.43251
<LVFFAEDVG+D	α1-9+β1-1	αb9+βb1	1075.51003
FAED+DAEFR>	α4-7+β1-5	αi4-7+βfull	1081.45906
<LVFFAEDV+DA	α1-8+β1-2	αb8+βb2	1089.52568
AEDVG+DAEFR>	α5-9+β1-5	αi5-9+βfull	1090.48052
FFAEDVGSNK>	α3-12	αy10	1095.5111
VFFAEDV+DAE	α2-8+β1-3	αi2-8+βb3	1105.48421
EDVGS+DAEFR>	α6-10+β1-5	αi6-10+βfull	1106.47544
FFAE+DAEFR>	α3-6+β1-5	αi3-6+βfull	1113.50053
AEDVGSNK>+DAE	α5-12+β1-3	αy8+βb3	1116.48092
FAEDVGSN+DAE	α4-11+β1-3	αi4-11+βb3	1117.44381
AEDVGSN+DAEF	α5-11+β1-4	αi5-11+βb4	1117.44381
<LVFFAED+DAE	α1-7+β1-3	αb7+βb3	1119.49986
VFFAEDVGS+DA	α2-10+β1-2	αi2-10+βb2	1120.49511
FAEDVGSNK>+DA	α4-12+β1-2	αy9+βb2	1134.50674
FFAEDVGSN+DA	α3-11+β1-2	αi3-11+βb2	1135.46963
<LVFFAEDVG+DA	α1-9+β1-2	αb9+βb2	1146.54715
FFAEDVGS+DAE	α3-10+β1-3	αi3-10+βb3	1150.46929
FAEDVGS+DAEF	α4-10+β1-4	αi4-10+βb4	1150.46929
<LVFFAE+DAEF	α1-6+β1-4	αb6+βb4	1151.54133
VFFAED+DAEF	α2-7+β1-4	αi2-7+βb4	1153.48421
FFAEDV+DAEF	α3-8+β1-4	αi3-8+βb4	1153.48421
<LVFFAEDVGSN	α1-11	αb11	1161.55805
VFFAEDVG+DAE	α2-9+β1-3	αi2-9+βb3	1162.50568
<LVFFAEDVGS+D	α1-10+β1-1	αb10+βb1	1162.54206
VFFAEDVGSN+D	α2-11+β1-1	αi2-11+βb1	1163.50093
AEDVGS+DAEFR>	α5-10+β1-5	αi5-10+βfull	1177.51255
FAEDV+DAEFR>	α4-8+β1-5	αi4-8+βfull	1180.52747
EDVGSNK>+DAEF	α6-12+β1-4	αy7+βb4	1192.51222
VFFAEDVGSNK>	α2-12	αy11	1194.57951

FFAEDVG+DAEF	α3-9+β1-4	αi3-9+βb4	1210.50568
FFAEDVGSNK>+D	α3-12+β1-1	αy10+βb1	1210.53804
VFFAE+DAEFR>	α2-6+β1-5	αi2-6+βfull	1212.56895
<LVFFAEDV+DAE	α1-8+β1-3	αb8+βb3	1218.56828
EDVGSN+DAEFR>	α6-11+β1-5	αi6-11+βfull	1220.51837
FFAED+DAEFR>	α3-7+β1-5	αi3-7+βfull	1228.52747
<LVFFAEDVGS+DA	α1-10+β1-2	αb10+βb2	1233.57918
VFFAEDVGSN+DA	α2-11+β1-2	αi2-11+βb2	1234.53804
FAEDVG+DAEFR>	α4-9+β1-5	αi4-9+βfull	1237.54894
VFFAEDVGS+DAE	α2-10+β1-3	αi2-10+βb3	1249.53771
VFFAEDV+DAEF	α2-8+β1-4	αi2-8+βb4	1252.55263
AEDVGSNK>+DAEF	α5-12+β1-4	αy8+βb4	1263.54933
FAEDVGSNK>+DAE	α4-12+β1-3	αy9+βb3	1263.54933
FFAEDVGSN+DAE	α3-11+β1-3	αi3-11+βb3	1264.51222
FAEDVGSN+DAEF	α4-11+β1-4	αi4-11+βb4	1264.51222
<LVFFAED+DAEF	α1-7+β1-4	αb7+βb4	1266.56828
<LVFFAEDVG+DAE	α1-9+β1-3	αb9+βb3	1275.58974
<LVFFAEDVGSN+D	α1-11+β1-1	αb11+βb1	1276.58499
FFAEDVGSNK>+DA	α3-12+β1-2	αy10+βb2	1281.57515
AEDVGSN+DAEFR>	α5-11+β1-5	αi5-11+βfull	1291.55548
FFAEDVGS+DAEF	α3-10+β1-4	αi3-10+βb4	1297.53771
<LVFFAEDVGSNK>	α1-12	αfull	1307.66357
VFFAEDVG+DAEF	α2-9+β1-4	αi2-9+βb4	1309.57409
VFFAEDVGSNK>+D	α2-12+β1-1	αy11+βb1	1309.60645
FAEDVGS+DAEFR>	α4-10+β1-5	αi4-10+βfull	1324.58097
<LVFFAE+DAEFR>	α1-6+β1-5	αb6+βfull	1325.65301
FFAEDV+DAEFR>	α3-8+β1-5	αi3-8+βfull	1327.59589
VFFAED+DAEFR>	α2-7+β1-5	αi2-7+βfull	1327.59589
<LVFFAEDVGSN+DA	α1-11+β1-2	αb11+βb2	1347.6221
<LVFFAEDVGS+DAE	α1-10+β1-3	αb10+βb3	1362.62177
VFFAEDVGSN+DAE	α2-11+β1-3	αi2-11+βb3	1363.58063
<LVFFAEDV+DAEF	α1-8+β1-4	αb8+βb4	1365.63669
EDVGSNK>+DAEFR>	α6-12+β1-5	αy7+βfull	1366.62389
VFFAEDVGSNK>+DA	α2-12+β1-2	αy11+βb2	1380.64357
FFAEDVG+DAEFR>	α3-9+β1-5	αi3-9+βfull	1384.61735
VFFAEDVGS+DAEF	α2-10+β1-4	αi2-10+βb4	1396.60612
FFAEDVGSNK>+DAE	α3-12+β1-3	αy10+βb3	1410.61775
FAEDVGSNK>+DAEF	α4-12+β1-4	αy9+βb4	1410.61775
FFAEDVGSN+DAEF	α3-11+β1-4	αi3-11+βb4	1411.58063
<LVFFAEDVG+DAEF	α1-9+β1-4	αb9+βb4	1422.65815

<LVFFAEDVGSNK>+D	α1-12+β1-1	αfull+βb1	1422.69052
VFFAEDV+DAEFR>	α2-8+β1-5	αi2-8+βfull	1426.6643
AEDVGSNK>+DAEFR>	α5-12+β1-5	αy8+βfull	1437.66101
FAEDVGSN+DAEFR>	α4-11+β1-5	αi4-11+βfull	1438.62389
<LVFFAED+DAEFR>	α1-7+β1-5	αb7+βfull	1440.67995
FFAEDVGS+DAEFR>	α3-10+β1-5	αi3-10+βfull	1471.64938
<LVFFAEDVGSN+DAE	α1-11+β1-3	αb11+βb3	1476.6647
VFFAEDVG+DAEFR>	α2-9+β1-5	αi2-9+βfull	1483.68577
<LVFFAEDVGSNK>+DA	α1-12+β1-2	αfull+βb2	1493.72763
VFFAEDVGSNK>+DAE	α2-12+β1-3	αy11+βb3	1509.68616
<LVFFAEDVGS+DAEF	α1-10+β1-4	αb10+βb4	1509.69018
VFFAEDVGSN+DAEF	α2-11+β1-4	αi2-11+βb4	1510.64905
<LVFFAEDV+DAEFR>	α1-8+β1-5	αb8+βfull	1539.74837
FFAEDVGSNK>+DAEF	α3-12+β1-4	αy10+βb4	1557.68616
VFFAEDVGS+DAEFR>	α2-10+β1-5	αi2-10+βfull	1570.71779
FAEDVGSNK>+DAEFR>	α4-12+β1-5	αy9+βfull	1584.72942
FFAEDVGSN+DAEFR>	α3-11+β1-5	αi3-11+βfull	1585.69231
<LVFFAEDVG+DAEFR>	α1-9+β1-5	αb9+βfull	1596.76983
<LVFFAEDVGSNK>+DAE	α1-12+β1-3	αfull+βb3	1622.77022
<LVFFAEDVGSN+DAEF	α1-11+β1-4	αb11+βb4	1623.73311
VFFAEDVGSNK>+DAEF	α2-12+β1-4	αy11+βb4	1656.75457
<LVFFAEDVGS+DAEFR>	α1-10+β1-5	αb10+βfull	1683.80186
VFFAEDVGSN+DAEFR>	α2-11+β1-5	αi2-11+βfull	1684.76072
FFAEDVGSNK>+DAEFR>	α3-12+β1-5	αy10+βfull	1731.79783
<LVFFAEDVGSNK>+DAEF	α1-12+β1-4	αfull+βb4	1769.83864
<LVFFAEDVGSN+DAEFR>	α1-11+β1-5	αb11+βfull	1797.84478
VFFAEDVGSNK>+DAEFR>	α2-12+β1-5	αy11+βfull	1830.86625
<LVFFAEDVGSNK>+DAEFR>	α1-12+β1-5	αfull+βfull	1943.95031

Amyloid-β17-28×1-5, –H_2O link

		β-chain label 1	**β1-1**	**β1-2**	**β1-3**	**β1-4**	**β1-5**	β2-2	β2-3	β2-4	**β2-5**	β3-3	β3-4	**β3-5**	β4-4	**β4-5**	**β5-5**
		β-chain label 2	**βb1**	**βb2**	**βb3**	**βb4**	**βfull (βy5)**	βi2	βi2-3	βi2-4	**βy4**	βi3	βi3-4	**βy3**	βi4	**βy2**	**βy1**
α-chain label 1	α-chain label 2		-D	-DA	-DAE	-DAEF	-DAEFR>	A	AE	AEF	AEFR>	E	EF	EFR>	F	FR>	R>
α1-1	**αb1**	<L															
α1-2	**αb2**	<LV															
α1-3	**αb3**	<LVF															
α1-4	**αb4**	<LVFF															
α1-5	**αb5**	<LVFFA							**Identified sequences**								
α1-6	**αb6**	<LVFFAE |	<LVFFAE | D	<LVFFAE | DA	<LVFFAE | DAE	<LVFFAE | DAEF	<LVFFAE | DAEFR>		Precursor								
α1-7	**αb7**	<LVFFAED |	<LVFFAED | D	<LVFFAED | DA	<LVFFAED | DAE	<LVFFAED | DAEF	<LVFFAED | DAEFR>		One bond cleaved								
α1-8	**αb8**	<LVFFAEDV |	<LVFFAEDV | D	<LVFFAEDV | DA	<LVFFAEDV | DAE	<LVFFAEDV | DAEF	<LVFFAEDV | DAEFR>		Two bonds cleaved								
α1-9	**αb9**	<LVFFAEDVG |	<LVFFAEDVG | D	<LVFFAEDVG | DA	<LVFFAEDVG | DAE	<LVFFAEDVG | DAEF	<LVFFAEDVG | DAEFR>		Three bonds cleaved								
α1-10	**αb10**	<LVFFAEDVGS |	<LVFFAEDVGS | D	<LVFFAEDVGS | DA	<LVFFAEDVGS | DAE	<LVFFAEDVGS | DAEF	<LVFFAEDVGS | DAEFR>										
α1-11	**αb11**	<LVFFAEDVGSN |	<LVFFAEDVGSN | D	<LVFFAEDVGSN | DA	<LVFFAEDVGSN | DAE	<LVFFAEDVGSN | DAEF	<LVFFAEDVGSN | DAEFR>										
α1-12	**αfull**	<LVFFAEDVGSNK> |	<LVFFAEDVGSNK> | D	<LVFFAEDVGSNK> | DA	<LVFFAEDVGSNK> | DAE	<LVFFAEDVGSNK> | DAEF	<LVFFAEDVGSNK> | DAEFR>										
α2-2	αi2	V															
α2-3	αi2-3	VF															
α2-4	αi2-4	VFF															
α2-5	αi2-5	VFFA															
α2-6	αi2-6	VFFAE |	VFFAE | D	VFFAE | DA	VFFAE | DAE	VFFAE | DAEF	VFFAE | DAEFR>										
α2-7	αi2-7	VFFAED |	VFFAED | D	VFFAED | DA	VFFAED | DAE	VFFAED | DAEF	VFFAED | DAEFR>										
α2-8	αi2-8	VFFAEDV |	VFFAEDV | D	VFFAEDV | DA	VFFAEDV | DAE	VFFAEDV | DAEF	VFFAEDV | DAEFR>										
α2-9	αi2-9	VFFAEDVG |	VFFAEDVG | D	VFFAEDVG | DA	VFFAEDVG | DAE	VFFAEDVG | DAEF	VFFAEDVG | DAEFR>										
α2-10	αi2-10	VFFAEDVGS |	VFFAEDVGS | D	VFFAEDVGS | DA	VFFAEDVGS | DAE	VFFAEDVGS | DAEF	VFFAEDVGS | DAEFR>										
α2-11	αi2-11	VFFAEDVGSN |	VFFAEDVGSN | D	VFFAEDVGSN | DA	VFFAEDVGSN | DAE	VFFAEDVGSN | DAEF	VFFAEDVGSN | DAEFR>										
α2-12	**αy11**	VFFAEDVGSNK> |	VFFAEDVGSNK> | D	VFFAEDVGSNK> | DA	VFFAEDVGSNK> | DAE	VFFAEDVGSNK> | DAEF	VFFAEDVGSNK> | DAEFR>										
α3-3	αi3	F															
α3-4	αi3-4	FF															
α3-5	αi3-5	FFA															

α3-6	αi3-6	FFAE |	FFAE | D	FFAE | DA	FFAE | DAE	FFAE | DAEF	FFAE | DAEFR>										
α3-7	αi3-7	FFAED |	FFAED | D	FFAED | DA	FFAED | DAE	FFAED | DAEF	FFAED | DAEFR>										
α3-8	αi3-8	FFAEDV |	FFAEDV | D	FFAEDV | DA	FFAEDV | DAE	FFAEDV | DAEF	FFAEDV | DAEFR>										
α3-9	αi3-9	FFAEDVG |	FFAEDVG | D	FFAEDVG | DA	FFAEDVG | DAE	FFAEDVG | DAEF	FFAEDVG | DAEFR>										
α3-10	αi3-10	FFAEDVGS |	FFAEDVGS | D	FFAEDVGS | DA	FFAEDVGS | DAE	FFAEDVGS | DAEF	FFAEDVGS | DAEFR>										
α3-11	αi3-11	FFAEDVGSN |	FFAEDVGSN | D	FFAEDVGSN | DA	FFAEDVGSN | DAE	FFAEDVGSN | DAEF	FFAEDVGSN | DAEFR>										
α3-12	**αy10**	FFAEDVGSNK> |	FFAEDVGSNK> | D	FFAEDVGSNK> | DA	FFAEDVGSNK> | DAE	FFAEDVGSNK> | DAEF	FFAEDVGSNK> | DAEFR>										
α4-4	αi4	F															
α4-5	αi4-5	FA															
α4-6	αi4-6	FAE |	FAE | D	FAE | DA	FAE | DAE	FAE | DAEF	FAE | DAEFR>										
α4-7	αi4-7	FAED |	FAED | D	FAED | DA	FAED | DAE	FAED | DAEF	FAED | DAEFR>										
α4-8	αi4-8	FAEDV |	FAEDV | D	FAEDV | DA	FAEDV | DAE	FAEDV | DAEF	FAEDV | DAEFR>										
α4-9	αi4-9	FAEDVG |	FAEDVG | D	FAEDVG | DA	FAEDVG | DAE	FAEDVG | DAEF	FAEDVG | DAEFR>										
α4-10	αi4-10	FAEDVGS |	FAEDVGS | D	FAEDVGS | DA	FAEDVGS | DAE	FAEDVGS | DAEF	FAEDVGS | DAEFR>										
α4-11	αi4-11	FAEDVGSN |	FAEDVGSN | D	FAEDVGSN | DA	FAEDVGSN | DAE	FAEDVGSN | DAEF	FAEDVGSN | DAEFR>										
α4-12	**αy9**	FAEDVGSNK> |	FAEDVGSNK> | D	FAEDVGSNK> | DA	FAEDVGSNK> | DAE	FAEDVGSNK> | DAEF	FAEDVGSNK> | DAEFR>										
α5-5	αi5	A															
α5-6	αi5-6	AE |	AE | D	AE | DA	AE | DAE	AE | DAEF	AE | DAEFR>										
α5-7	αi5-7	AED |	AED | D	AED | DA	AED | DAE	AED | DAEF	AED | DAEFR>										
α5-8	αi5-8	AEDV |	AEDV | D	AEDV | DA	AEDV | DAE	AEDV | DAEF	AEDV | DAEFR>										
α5-9	αi5-9	AEDVG |	AEDVG | D	AEDVG | DA	AEDVG | DAE	AEDVG | DAEF	AEDVG | DAEFR>										
α5-10	αi5-10	AEDVGS |	AEDVGS | D	AEDVGS | DA	AEDVGS | DAE	AEDVGS | DAEF	AEDVGS | DAEFR>										
α5-11	αi5-11	AEDVGSN |	AEDVGSN | D	AEDVGSN | DA	AEDVGSN | DAE	AEDVGSN | DAEF	AEDVGSN | DAEFR>										
α5-12	**αy8**	AEDVGSNK> |	AEDVGSNK> | D	AEDVGSNK> | DA	AEDVGSNK> | DAE	AEDVGSNK> | DAEF	AEDVGSNK> | DAEFR>										
α6-6	αi6	E |	E | D	E | DA	E | DAE	E | DAEF	E | DAEFR>										
α6-7	αi6-7	ED |	ED | D	ED | DA	ED | DAE	ED | DAEF	ED | DAEFR>										
α6-8	αi6-8	EDV |	EDV | D	EDV | DA	EDV | DAE	EDV | DAEF	EDV | DAEFR>										
α6-9	αi6-9	EDVG |	EDVG | D	EDVG | DA	EDVG | DAE	EDVG | DAEF	EDVG | DAEFR>										
α6-10	αi6-10	EDVGS |	EDVGS | D	EDVGS | DA	EDVGS | DAE	EDVGS | DAEF	EDVGS | DAEFR>										
α6-11	αi6-11	EDVGSN |	EDVGSN | D	EDVGSN | DA	EDVGSN | DAE	EDVGSN | DAEF	EDVGSN | DAEFR>										
α6-12	**αy7**	EDVGSNK> |	EDVGSNK> | D	EDVGSNK> | DA	EDVGSNK> | DAE	EDVGSNK> | DAEF	EDVGSNK> | DAEFR>										
α7-7	αi7	D															
α7-8	αi7-8	DV															

α7-9	αi7-9	DVG															
α7-10	αi7-10	DVGS															
α7-11	αi7-11	DVGSN															
α7-12	**αy6**	DVGSNK>															
α8-8	αi8	V															
α8-9	αi8-9	VG															
α8-10	αi8-10	VGS															
α8-11	αi8-11	VGSN															
α8-12	**αy5**	VGSNK>															
α9-9	αi9	G															
α9-10	αi9-10	GS															
α9-11	αi9-11	GSN															
α9-12	**αy4**	GSNK>															
α10-10	αi10	S															
α10-11	αi10-11	SN															
α10-12	**αy3**	SNK>															
α11-11	αi11	N															
α11-12	αy2	NK>															
α12-12	αy1	K>															

PEAKS Studio MS/MS		
m/z=972.4794		
Charge=2+		
RT=36.8 min		
Deconvoluted [M+H]+	Signal	Identification [≤20 ppm]
101.107574	3.22E+05	
112.086945	3.81E+05	
113.07096	6.48E+04	
115.08658	1.50E+05	
116.07081	3.65E+05	
120.080956	1.28E+07	
121.0842	1.20E+05	
129.10211	9.04E+06	
130.08624	1.78E+06	αy1-NH3
130.09749	9.26E+04	
133.06064	1.52E+05	
145.06055	2.09E+05	
147.1126	3.39E+06	αy1
153.12479	9.54E+04	
157.09673	2.76E+05	
157.1084	2.35E+05	
167.09242	8.76E+04	
175.11877	4.77E+06	βy1
185.16461	1.15E+07	
187.10728	3.07E+05	
190.09734	2.92E+05	
191.11792	1.33E+05	
198.12387	1.58E+05	
205.10083	3.74E+05	
208.108	1.11E+05	
209.09174	6.33E+05	
213.098	7.84E+04	
213.15948	1.50E+07	αb2
215.10233	3.39E+05	
219.11256	2.74E+05	αi4-5
219.14876	5.68E+05	
225.13422	9.48E+04	
226.11824	2.82E+06	
227.10254	2.06E+05	

239.175	1.60E+05	
241.09286	2.42E+05	
242.07675	1.79E+05	
244.12889	2.59E+06	αy2-NH3
247.14372	1.04E+06	αi2-3
259.10315	4.35E+05	
261.15527	6.81E+06	αy2
265.1545	1.23E+05	
267.1489	3.94E+06	
272.12378	2.19E+05	
284.19647	3.61E+05	
287.21136	2.15E+05	
295.14368	2.91E+06	αi3-4
296.12347	1.28E+05	
305.1601	1.69E+06	βy2-NH3
312.1661	1.18E+05	
313.14978	1.13E+06	
315.1769	8.35E+05	
315.20593	2.13E+06	
316.11353	1.40E+05	
316.2096	1.25E+05	
322.18695	2.06E+07	βy2
330.1767	6.31E+05	αy3-H2O
331.16046	7.69E+05	αy3-NH3
332.1963	2.83E+05	
340.15964	1.96E+05	
341.14502	2.40E+05	
348.18732	5.97E+06	αy3
352.16125	6.74E+05	
358.17108	4.36E+05	
359.15527	4.75E+05	
360.2276	9.22E+06	αb3
366.18066	1.89E+06	αi3-5
367.2082	1.21E+05	
369.1875	3.35E+05	
370.17114	1.52E+06	
376.18207	1.45E+05	αi8-11
382.12366	2.02E+05	
386.2432	3.29E+05	

387.198	2.28E+06	αy4-H2O
388.18198	1.11E+06	αy4-NH3
394.21188	9.98E+05	αi2-4
403.1556	2.94E+05	
403.2699	1.85E+05	
405.20862	1.82E+07	αy4
408.22882	2.58E+05	
413.12933	1.79E+05	αi6-7+βb2; αi5-7+βb1
416.19305	2.45E+05	
422.20618	2.01E+05	
431.26437	5.88E+05	
433.21878	4.27E+05	βy3-H2O
434.2027	1.64E+05	βy3-NH3
445.172	1.94E+05	αi4-7+β-; αi4-6+βb1
451.2298	3.98E+06	βy3
451.26917	2.55E+05	
455.1891	1.40E+05	
456.17285	1.78E+05	
462.2735	2.42E+05	
465.24854	7.50E+05	αi2-5
469.23993	3.30E+05	
473.20023	1.23E+05	
474.18207	2.92E+05	
479.2649	9.49E+05	
479.30112	1.73E+06	
486.2664	9.44E+05	αy5-H2O
487.22995	1.59E+05	
487.25137	7.50E+05	αy5-NH3
493.24396	2.38E+05	
504.2771	1.59E+07	αy5
505.24246	3.15E+05	βy4-NH3
507.2959	1.32E+06	αb4
522.2665	2.78E+07	βy4
529.1936	1.53E+05	
532.2517	8.02E+04	
533.3113	4.19E+05	
542.17334	1.27E+05	αi6-7+βb3
550.3382	6.89E+05	
557.25287	7.60E+04	
560.19684	7.34E+04	αi4-7+βb1

566.2563	5.87E+04	
578.3329	7.15E+05	αb5
584.26794	2.53E+05	
592.2392	1.93E+05	αi3-7+β-; αi3-6+βb1
601.29346	5.20E+05	αy6-H2O
602.256	2.77E+05	
602.27783	5.55E+05	αy6-NH3
619.3032	7.58E+06	αy6
620.2666	7.54E+05	βy5-NH3
637.29285	4.58E+06	βy5
703.30273	1.56E+06	
707.267	3.12E+05	αi3-7+βb1
710.3287	2.62E+05	
710.81805	2.68E+05	
729.3535	8.24E+04	
730.33594	3.31E+05	αy7+β-
748.32544	1.54E+05	αi6+βfull; αi3-9+β-
756.37756	1.87E+05	
783.3616	1.09E+05	
792.31805	2.13E+05	αi3-6+βb3; αi4-6+βb4
802.33765	2.25E+05	αi5-6+βfull-NH3; αi4-11+β-
804.3911	3.53E+05	αb7+β-; αb6+βb1
806.3345	2.04E+05	αi3-8+βb1; αi2-7+βb1
819.36176	6.58E+05	αi5-6+βfull
827.3511	2.15E+05	
833.3989	2.46E+05	
839.87964	1.33E+05	
845.36285	3.24E+05	αi3-9+βb1-H2O; αy7+βb1
847.3613	1.21E+05	
848.39246	1.45E+05	
849.3845	1.53E+05	
858.3921	2.83E+05	
863.3517	2.13E+06	αi6-7+βfull; αi3-9+βb1
866.90234	1.32E+06	
880.3805	1.41E+05	
917.40076	1.92E+05	
919.4206	2.87E+05	αb7+βb1
921.42786	2.15E+05	
934.389	3.18E+06	αi5-7+βfull; αi3-9+βb2
944.4397	2.10E+05	

955.463	3.91E+05	
962.4217	3.64E+05	αi6-8+βfull; αi2-9+βb1
966.4285	9.49E+05	αi4-6+βfull
972.3748	9.18E+04	
1005.46375	2.21E+05	
1006.41315	6.45E+04	
1009.47626	7.82E+04	
1018.4907	3.10E+05	αb8+βb1
1019.44055	2.45E+05	αi6-9+βfull
1027.4294	5.32E+04	
1033.4595	7.15E+05	αi5-8+βfull; αi2-9+βb2
1034.4602	9.27E+03	
1045.4424	3.62E+05	αy7+βb3
1047.44	3.53E+04	
1063.469	4.65E+05	αi4-7+βfull-H2O; αy9+βb1
1064.4692	5.41E+04	
1078.4832	4.74E+04	
1081.457	3.87E+06	αi4-7+βfull
1082.4604	1.28E+05	
1085.5037	2.01E+05	
1086.5061	1.76E+04	
1089.5186	4.27E+04	
1090.4724	4.48E+05	αi5-9+βfull
1091.4817	1.36E+04	
1095.5039	8.14E+04	
1098.4795	1.81E+05	
1106.4731	2.63E+05	αi6-10+βfull
1107.4788	1.43E+04	
1113.4971	1.94E+06	αi3-6+βfull
1116.4795	3.24E+05	αy8+βb3
1119.4937	2.59E+05	αb7+βb3
1123.4962	5.81E+04	
1132.5195	8.42E+04	
1135.504	1.55E+05	
1144.5234	5.26E+04	
1152.5286	8.41E+05	
1156.5383	1.37E+05	
1159.5007	1.43E+05	

1160.4993	3.28E+03	
1168.4946	6.38E+04	
1174.4988	4.79E+04	
1177.5121	3.54E+05	αi5-10+βfull
1180.5271	1.17E+06	αi4-8+βfull
1181.5264	1.10E+04	
1192.5176	5.10E+05	αy7+βb4
1193.5164	2.60E+04	
1194.5295	1.19E+05	
1202.5048	8.71E+04	
1203.4979	7.20E+04	
1210.5359	1.53E+06	αi3-7+βfull-H2O; αy10+βb1
1212.5657	2.59E+05	αi2-6+βfull
1214.5757	1.95E+04	
1220.5144	3.08E+05	αi6-11+βfull; αi4-9+βfull-NH3
1221.5005	5.50E+05	
1222.5092	1.61E+04	
1228.5247	1.04E+07	αi3-7+βfull
1236.544	7.52E+04	
1237.547	4.15E+05	αi4-9+βfull
1238.5361	5.14E+05	
1239.5282	4.96E+05	
1240.5312	5.57E+03	
1245.5482	2.88E+05	αy9+βb3-H2O; αy8+βb4-H2O
1246.5537	4.28E+04	
1247.5442	5.00E+04	
1263.5516	1.16E+06	αy9+βb3; αy8+βb4; αy10+βb2-H2O
1273.542	1.42E+05	αi5-11+βfull-H2O
1274.5323	9.21E+04	αi5-11+βfull-NH3
1281.5703	1.69E+05	αy10+βb2
1282.5737	2.29E+05	
1291.5488	3.98E+05	αi5-11+βfull; αi2-9+βb4-H2O
1292.5448	1.08E+06	
1297.6564	2.66E+06	
1298.6592	1.09E+05	
1299.5947	1.34E+06	
1307.6559	2.80E+05	αb6+βfull-H2O; αfull+β-
1309.5668	5.85E+05	αi2-9+βb4; αi3-8+βfull-H2O; αi2-

		7+βfull-H2O
1310.5605	4.06E+05	αi3-8+βfull-NH3; αi2-7+βfull-NH3
1324.5757	2.01E+05	αi4-10+βfull
1325.6506	7.05E+06	αb6+βfull
1326.6534	3.36E+05	
1327.5912	4.81E+06	αi3-8+βfull; αi2-7+βfull
1331.5798	4.16E+05	
1342.6659	4.18E+05	
1343.669	2.45E+05	
1348.6091	8.00E+05	αy7+βfull-H2O
1349.6013	2.94E+06	αy7+βfull-NH3
1366.6213	1.45E+07	αi3-9+βfull-H2O; αy7+βfull
1367.6248	2.72E+05	
1368.6926	4.43E+05	
1369.705	4.91E+05	
1377.6248	1.89E+05	
1384.6143	1.52E+06	αi3-9+βfull
1402.6284	6.12E+05	
1404.6761	3.82E+05	αfull+βb1-H2O
1405.6792	2.47E+05	αfull+βb1-NH3
1410.6161	1.76E+06	αy10+βb3; αy9+βb4
1419.65	9.71E+05	αy8+βfull-H2O
1420.6381	3.02E+06	αy8+βfull-NH3
1422.6897	8.55E+06	αb7+βfull-H2O; αfull+βb1
1423.6927	1.07E+06	
1426.6597	5.50E+05	αi2-8+βfull
1437.6595	2.09E+07	αy8+βfull
1438.6625	1.85E+05	
1439.6578	1.55E+06	
1440.6779	3.20E+07	αb7+βfull
1441.6808	1.05E+06	
1444.6793	1.96E+05	
1453.6361	5.35E+05	αi3-10+βfull-H2O
1454.6377	3.18E+03	
1455.6428	9.05E+04	
1456.6332	9.23E+05	
1457.636	5.55E+03	
1471.6467	1.35E+06	αi3-10+βfull
1472.6498	2.18E+05	
1483.6836	1.30E+05	αi2-9+βfull

1484.6866	6.99E+04	
1488.6654	2.74E+05	
1489.6685	7.59E+04	
1493.7245	8.79E+05	αfull+βb2
1494.7313	6.13E+04	
1495.7344	3.46E+04	
1510.686	5.86E+04	
1511.7524	2.46E+06	
1523.7208	5.58E+04	
1527.7202	5.44E+04	
1539.7456	1.11E+07	αb8+βfull
1540.7502	8.28E+05	
1548.694	2.23E+05	
1549.6895	4.25E+05	
1553.7783	1.07E+05	
1557.687	7.76E+05	αy10+βb4
1559.6925	3.32E+04	
1566.7214	1.92E+06	αy9+βfull-H2O
1567.7048	1.99E+06	αy9+βfull-NH3
1568.6936	1.25E+06	
1569.7727	2.86E+05	
1579.7554	6.60E+04	
1584.727	2.72E+07	αy9+βfull
1587.6802	8.85E+05	
1594.7731	2.94E+05	
1595.7761	4.07E+04	
1596.7655	6.71E+06	αb9+βfull
1597.7686	5.12E+05	
1603.7028	6.13E+05	
1604.6903	7.76E+05	
1606.7424	1.95E+05	
1614.7795	2.39E+05	
1622.7677	4.45E+06	αfull+βb3
1623.7703	8.59E+04	
1638.7766	2.34E+05	
1653.7899	1.60E+05	
1654.793	1.88E+04	
1655.808	1.88E+06	
1656.811	8.06E+04	
1665.7914	1.30E+06	αb10+βfull-H2O

1667.7941	3.70E+04	
1672.7594	1.01E+05	
1683.7994	4.31E+06	αb10+βfull
1684.8025	3.92E+05	
1696.7573	1.57E+06	
1697.7554	1.41E+04	
1698.7504	2.04E+05	
1700.8257	3.38E+05	
1713.783	4.65E+06	αy10+βfull-H2O
1714.7754	6.26E+06	αy10+βfull-NH3
1731.7946	6.12E+07	αy10+βfull
1732.7976	3.54E+05	
1741.8433	6.57E+04	
1742.8424	1.24E+05	
1743.8455	1.82E+04	
1751.8202	1.15E+05	αfull+βb4-H2O
1752.8232	3.11E+04	
1769.8405	1.69E+06	αfull+βb4
1770.8435	1.74E+05	
1779.8291	4.83E+05	αb11+βfull-H2O
1781.8257	9.39E+04	
1787.8423	2.60E+05	
1797.8363	4.38E+06	αb11+βfull
1798.8394	1.54E+06	
1812.8387	6.00E+05	αy11+βfull-H2O
1813.8418	5.43E+05	αy11+βfull-NH3
1814.8547	6.39E+04	
1815.8531	2.68E+06	
1816.8562	1.39E+05	
1830.8601	9.29E+06	αy11+βfull
1839.8419	7.15E+05	
1907.9122	2.16E+06	
1925.9313	1.45E+07	Precursor-H2O
1926.9303	7.48E+05	Precursor-NH3
1943.9463	1.89E+08	Precursor