Supporting Information for:

Separation of β-Amyloid Tryptic Peptide Species with Isomerized and Racemized L-Aspartic Residues with Ion Mobility in Structures for Lossless Ion Manipulations

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1) LVFFAE**D**VGS**D**K[+8]	L-Asp, L-Asp
2) LVFFAE**D**VGS**(dD)**K[+8]	L-Asp, D-Asp
3) LVFFAE**D**VGS**(bD)**K[+8]	L-Asp, L-isoAsp
4) LVFFAE**D**VGS**(dbD)**K[+8]	L-Asp, D-isoAsp

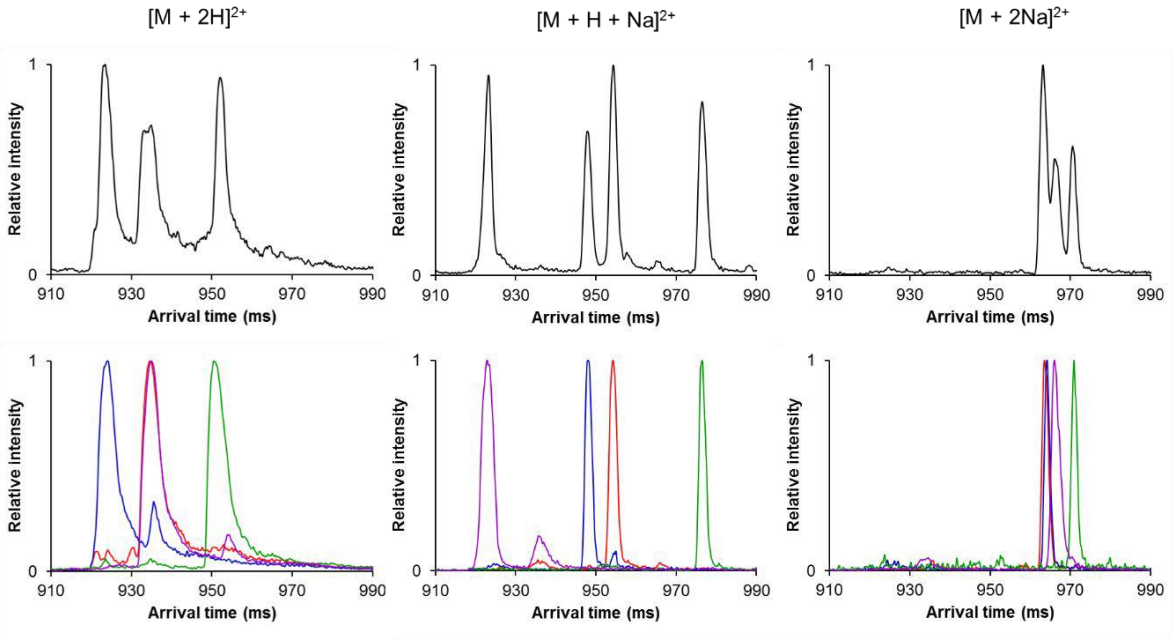

Figure S1. 72 m SLIM SUPER IM separation of Aβ peptide epimers 1-4. All conditions were the same as those described in the experimental section.

5) LVFFAE**(dD)**VGS**D**K[+8]	D-Asp, L-Asp
6) LVFFAE**(dD)**VGS**(dD)**K[+8]	D-Asp, D-Asp
7) LVFFAE**(dD)**VGS**(bD)**K[+8]	D-Asp, L-isoAsp
8) LVFFAE**(dD)**VGS**(dbD)**K[+8]	D-Asp, D-isoAsp

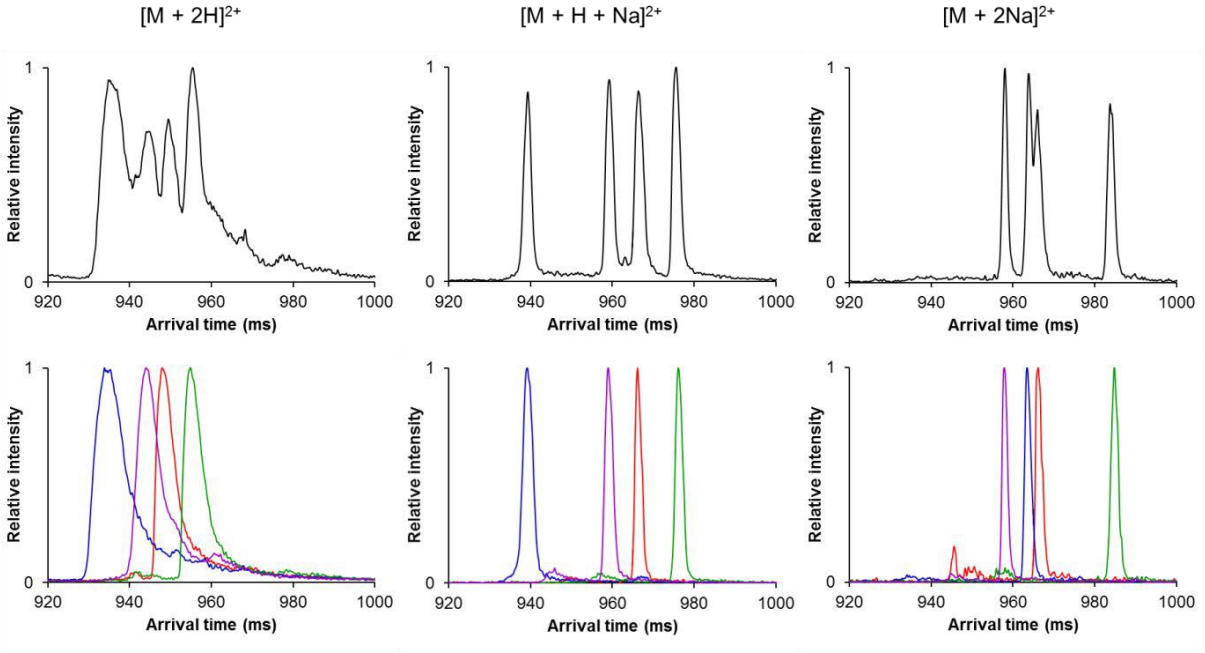

Figure S2. 72 m SLIM SUPER IM separation of Aβ peptide epimers 5-8. All conditions were the same as those described in the experimental section.

9) LVFFAE**(bD)**VGS**D**K[+8]	L-isoAsp, L-Asp
10) LVFFAE**(bD)**VGS**(dD)**K[+8]	L-isoAsp, D-Asp
11) LVFFAE**(bD)**VGS**(bD)**K[+8]	L-isoAsp, L-isoAsp
12) LVFFAE**(bD)**VGS**(dbD)**K[+8]	L-isoAsp, D-isoAsp

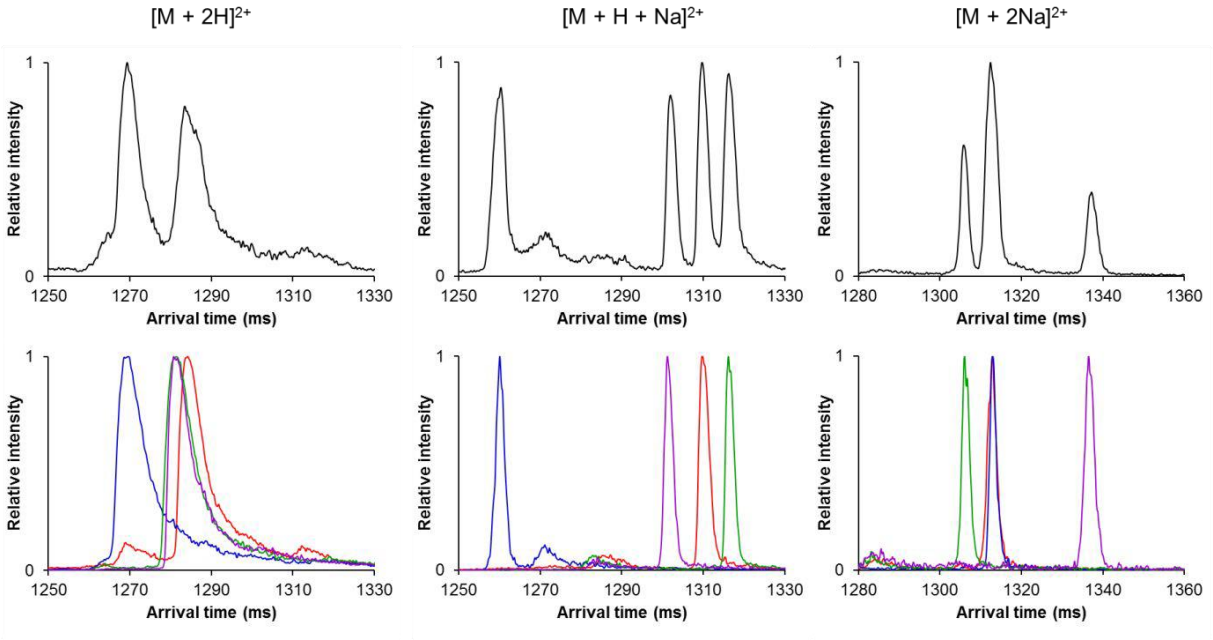

Figure S3. 99 m SLIM SUPER IM separation of Aβ peptide epimers 9-12. All conditions were the same as those described in the experimental section.

13) LVFFAE**(dbD)**VGS**D**K[+8]	D-isoAsp, L-Asp
14) LVFFAE**(dbD)**VGS**(dD)**K[+8]	D-isoAsp, D-Asp
15) LVFFAE**(dbD)**VGS**(bD)**K[+8]	D-isoAsp, L-isoAsp
16) LVFFAE**(dbD)**VGS**(dbD)**K[+8]	D-isoAsp, D-isoAsp

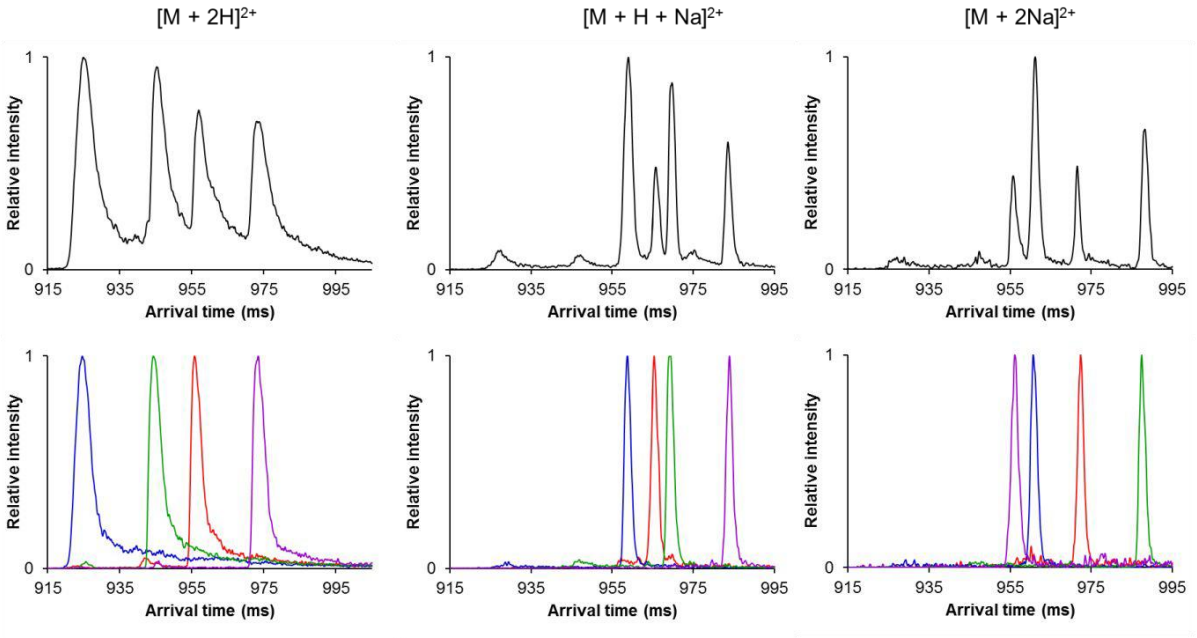

Figure S4. 72 m SLIM SUPER IM separation of Aβ peptide epimers 13-16. All conditions were the same as those described in the experimental section.

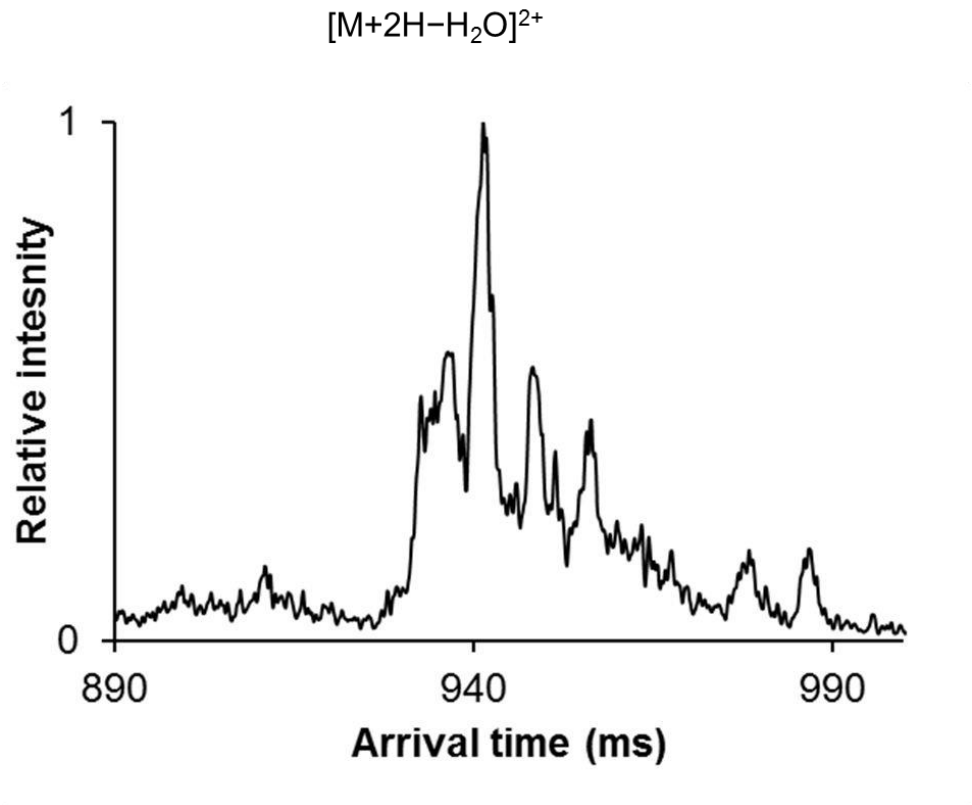

Figure S5. 72 m SLIM SUPER IM separation of Aβ peptide epimer 5-8 mixture. The dehydrated adducts each exhibit multiple conformations for each peptide.

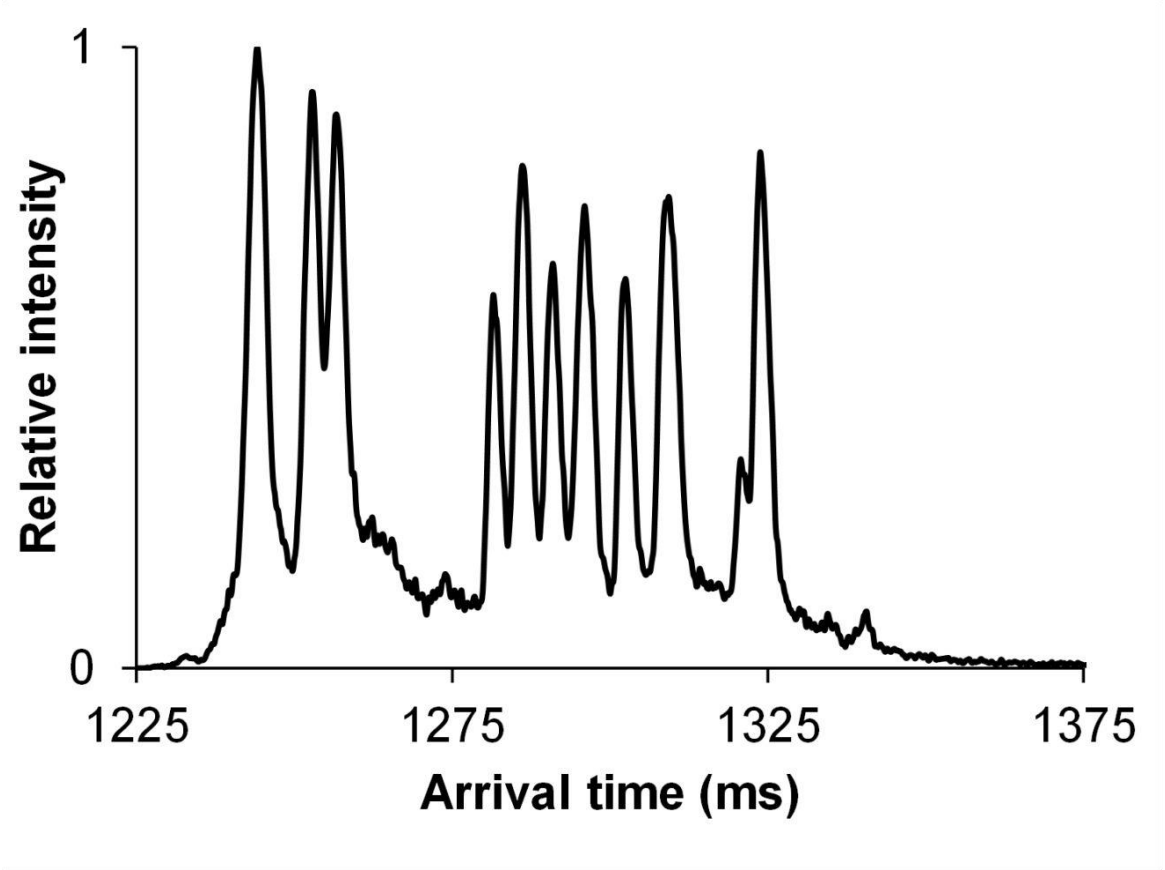

Figure S6. 99 m SLIM SUPER IM separation of a mixture of all 16 Aβ peptides as their $[M+H+Na]^{2+}$ adducts. Future work is ongoing in coupling our SLIM SUPER IM separations to a front-end LC separation to resolve all 16 possible Aβ17-28 peptides.

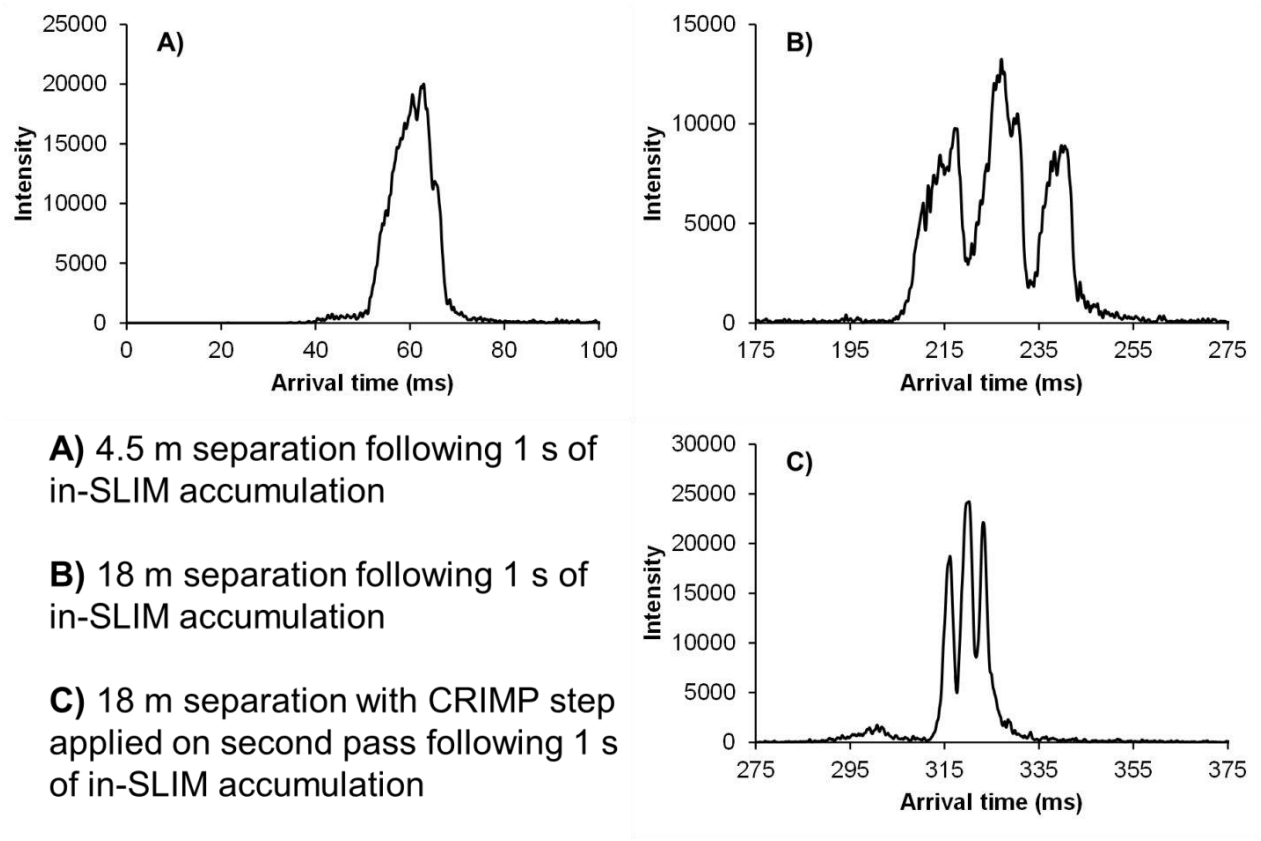

Figure S7. Demonstration of benefit of CRIMP step on improving S/N as well as overcoming the inherently broad peak widths associated with accumulating 1 s of ions during in-SLIM accumulation for epimer set 1-4. It is also seen that 18 m of separation is insufficient for their baseline resolution; baseline separation was achieved after 72 m (Figure 4B, manuscript) as $[M+H+Na]^{2+}$. Legend is located in bottom left corner of the figure. 5 individual SLIM SUPER IM separations were summed to produce each IM separation shown.

name	RT (min)	sequence with D/N forms	D/N forms
bA1728_1	25.66	LVFFAEDVGSDK	L-Asp, L-Asp
bA1728_2	25.89	LVFFAEDVGS(dD)K	L-Asp, D-Asp
bA1728_3	26.21	LVFFAEDVGS(bD)K	L-Asp, L-isoAsp
bA1728_4	26.27	LVFFAEDVGS(dbD)K	L-Asp, D-isoAsp
bA1728_5	25.33	LVFFAE(dD)VGSDK	D-Asp, L-Asp
bA1728_6	25.33	LVFFAE(dD)VGS(dD)K	D-Asp, D-Asp
bA1728_7	25.61	LVFFAE(dD)VGS(bD)K	D-Asp, L-isoAsp
bA1728_8	25.55	LVFFAE(dD)VGS(dbD)K	D-Asp, D-isoAsp
bA1728_9	25.61	LVFFAE(bD)VGSDK	L-isoAsp, L-Asp
bA1728_10	25.66	LVFFAE(bD)VGS(dD)K	L-isoAsp, D-Asp
bA1728_11	25.72	LVFFAE(bD)VGS(bD)K	L-isoAsp, L-isoAsp
bA1728_12	25.77	LVFFAE(bD)VGS(dbD)K	L-isoAsp, D-isoAsp
bA1728_13	26.05	LVFFAE(dbD)VGSDK	D-isoAsp, L-Asp
bA1728_14	26	LVFFAE(dbD)VGS(dD)K	D-isoAsp, D-Asp
bA1728_15	24.29	LVFFAE(dbD)VGS(bD)K	D-isoAsp, L-isoAsp
bA1728_16	25.83	LVFFAE(dbD)VGS(dbD)K	D-isoAsp, D-isoAsp

Figure S8. Peptide retention times under a 90 minute reversed-phase LC gradient with a Waters C18 column (100 µm i.d. × 10 cm, 1.7 µm BEH particles) at 40 °C. Mobile phase: A) water (0.5% formic acid), B) acetonitrile (0.5% formic acid). Gradient: 0 min, 0.5% B, 0.500 µL/min; 11 min, 0.5% B, 0.500 µL/min; 11.5 min, 0.5% B, 0.400 µL/min; 13 min, 0.5% B, 0.400 µL/min; 13.5 min, 5% B, 0.400 µL/min; 63.5 min, 30% B, 0.400 µL/min; 65 min, 95% B, 0.500 µL/ min; 80 min, 95% B, 0.500 µL/min; 83 min, 0.5% B, 0.500 µL/min.

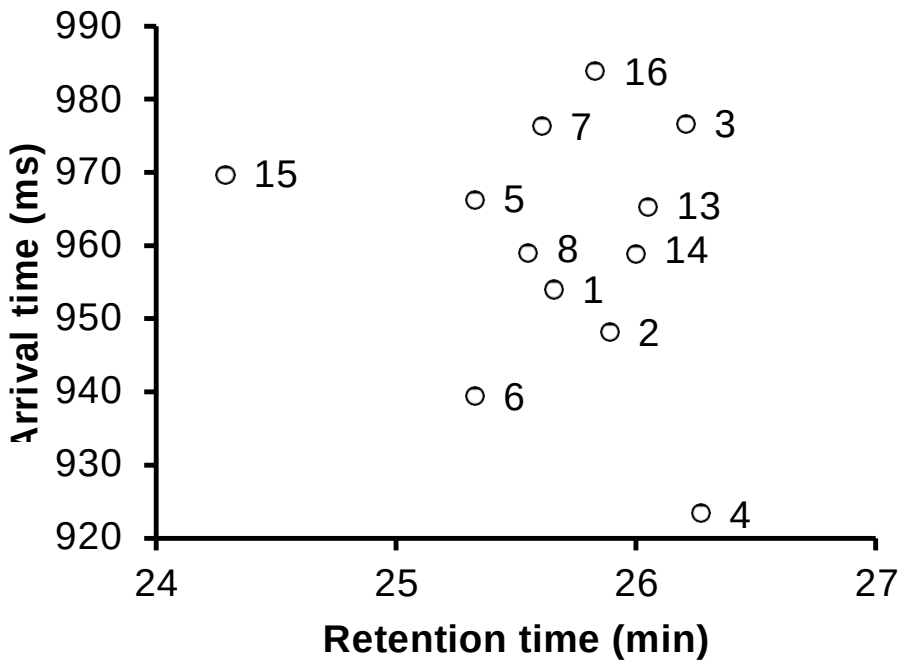

Figure S9. 2-D plot of peptides subjected to 72 m of SLIM SUPER IM separation, with their individual LC retention times on the x-axis and individual arrival times on the y-axis. Peptides 9-12 were not included since they required 99 m of SLIM SUPER IM separation to be fully resolved.