

Supplementary Data

Mass Spectrometric Characterization of Amyloid- β Species in the 7PA2 Cell Model of Alzheimer's Disease

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Supplementary Table 1
Endogenous A β PP/A β peptides detected in 7PA2 cell medium, which was immunodepleted by 82E1 and subsequently immunoprecipitated by 6E10 or 4G8, using nanoflow ESI-FTICR-MS/MS

Peptide	Theoretical mass [Da]	Δm [ppm] ^a	MS/MS ^b	Effect of BACE1 inhibition ^c
A β PP/A β _{-61 to 15}	8387.939	+1.6	Y	↑
A β PP/A β _{-61 to 39}	10790.242	-0.3		↑
A β PP/A β _{-61 to 40}	10889.311	-0.4		↑
A β PP/A β _{-45 to 15}	6601.144	+1.6	Y	↑
A β PP/A β _{-44 to 15}	6486.117	+2.4	Y	↑
A β PP/A β _{-44 to 38}	8789.352	+2.6		↑
A β PP/A β _{-44 to 39}	8888.420	+3.3		↑
A β PP/A β _{-44 to 40}	8987.489	+1.7		↑
A β PP/A β _{-39 to 15}	6017.884	+1.9	Y	↑
A β PP/A β _{-39 to 38}	8321.119	+2.5		↑
A β PP/A β _{-39 to 39}	8420.187	+2.4		↑
A β PP/A β _{-39 to 40}	8519.255	+2.9	Y	↑
A β PP/A β _{-39 to 42}	8703.377	+0.8		↑
A β PP/A β _{-36 to 15}	5673.751	+0.7		↑
A β PP/A β _{-36 to 38}	7976.985	+3.6		↑
A β PP/A β _{-36 to 39}	8076.054	+0.3	Y	↑
A β PP/A β _{-36 to 40}	8175.122	+2.1		↑
A β PP/A β _{-30 to 15}	5005.449	+0.1	Y	↑
A β PP/A β _{-30 to 39}	7407.752	+0.0		↑
A β PP/A β _{-30 to 40}	7506.821	+4.0		↑
A β PP/A β _{-25 to 15}	4539.184	+1.5	Y	→
A β PP/A β _{-25 to 38}	6842.418	+1.6		↑
A β PP/A β _{-25 to 39}	6941.487	+0.2		→
A β PP/A β _{-25 to 40}	7040.555	+3.2		↑
A β PP/A β _{-20 to 15}	3996.902	+2.3		↓
A β PP/A β _{-20 to 28}	5431.653	+1.7		↑
A β PP/A β _{-20 to 38}	6300.137	+2.1		↑
A β PP/A β _{-20 to 39}	6399.206	+2.6	Y	↑
A β PP/A β _{-20 to 40}	6498.274	+1.6	Y	↑
A β PP/A β _{-12 to 15}	3227.494	-1.0	Y	↑
A β PP/A β _{-12 to 19}	3714.810	+0.1	Y	↑
A β PP/A β _{-12 to 27}	4534.150	+2.3	Y	↑
A β PP/A β _{-12 to 28}	4662.245	+0.5	Y	↑
A β PP/A β _{-12 to 38}	5530.729	+1.7		↑
A β PP/A β _{-12 to 39}	5629.797	-1.7		↑
A β PP/A β _{-12 to 40}	5728.866	+1.7		↑
A β PP/A β _{-11 to 15}	3113.451	-1.0		↑
A β PP/A β _{-11 to 38}	5416.686	+2.4		↑
A β PP/A β _{-11 to 39}	5515.754	+2.3		↑
A β PP/A β _{-11 to 40}	5614.823	+1.8		↑
A β PP/A β _{-6 to 15}	2513.139	-0.6	Y	→
A β PP/A β _{-6 to 38}	4816.374	+0.6		↑
A β PP/A β _{-6 to 39}	4915.443	+4.3		↑
A β PP/A β _{-6 to 40}	5014.511	+1.5		↑
A β PP/A β _{-3 to 13}	1918.863	+0.2		↑
A β PP/A β _{-3 to 14}	2055.922	-0.2		↑
A β PP/A β _{-3 to 15}	2183.981	+0.2	Y	↑
A β PP/A β _{-3 to 17}	2425.160	-0.8		↑
A β PP/A β _{-3 to 18}	2524.228	-0.2		↑
A β PP/A β _{-3 to 19}	2671.297	-0.3	Y	↑
A β PP/A β _{-3 to 20}	2818.365	+0.0		↑
A β PP/A β _{-3 to 38}	4487.215	+1.8		↑
A β PP/A β _{-3 to 39}	4586.284	+2.0		↑
A β PP/A β _{-3 to 40}	4685.352	+1.5	Y	↑
A β PP/A β _{-3 to 42}	4869.473	+2.2		↑
A β ₁₋₁₃	1560.659	+0.3		→
A β ₁₋₁₄	1697.718	+0.2		→
A β ₁₋₁₅	1825.777	-0.6	Y	→

Supplementary Table 1
(Continued)

Peptide	Theoretical mass [Da]	Δm [ppm] ^a	MS/MS ^b	Effect of BACE1 inhibition ^c
A β ₁₋₁₇	2066.956	-0.1	Y	↓
A β ₁₋₁₈	2166.024	+0.3	Y	↓
A β ₁₋₁₉	2313.093	-1.9	Y	↓
A β ₁₋₂₀	2460.161	-1.2	Y	↓
A β ₁₋₂₇	3132.433	-0.7	Y	↓
A β ₁₋₂₈	3260.528	-1.0		→
A β ₁₋₂₉	3317.549	-0.6	Y	→
A β ₁₋₃₀	3388.586	-1.1		↓
A β ₁₋₃₁	3501.670	-1.6		↓
A β ₁₋₃₂	3614.754	+0.7	Y	↓
A β ₁₋₃₃	3671.776	-0.4	Y	↓
A β ₁₋₃₄	3784.860	+1.0	Y	↓
A β ₁₋₃₇	4071.990	+0.9	Y	→
A β ₁₋₃₈	4129.012	+2.1	Y	↓
A β ₁₋₃₉	4228.080	+0.1	Y	→
A β ₁₋₄₀	4327.148	+1.7	Y	→
A β ₁₋₄₁	4440.232	+2.5	Y	↓
A β ₁₋₄₂	4511.270	+1.8	Y	→
A β ₃₋₁₇	1880.892	-1.0		↓
A β ₃₋₂₀	2274.097	-0.5	Y	↓
A β ₅₋₂₉	2855.374	-0.9	Y	↑
A β ₅₋₃₃	3209.601	-0.5	Y	↑
A β ₅₋₃₈	3666.837	+0.9		↑
A β ₅₋₃₉	3765.905	+0.4		↑
A β ₅₋₄₀	3864.973	+1.5	Y	↑
A β ₅₋₄₁	3978.057	+2.6		↑
A β ₅₋₄₂	4049.095	+4.4	Y	↑
A β ₁₁₋₃₄	2607.381	+0.9	Y	↓
A β ₁₁₋₃₈	2951.533	+0.4		↓
A β ₁₁₋₃₉	3050.601	+2.8		↓
A β ₁₁₋₄₀	3149.670	+2.3	Y	↓
A β ₁₁₋₄₂	3333.791	+1.3		↓
A β ₁₇₋₃₈	2193.150	-0.5		↑
A β ₁₇₋₃₉	2292.219	+3.5	Y	↑
A β ₁₇₋₄₀	2391.287	+1.9		↑

^a Δm denotes the relative experimental mass deviation, $\Delta m = (m_{\text{exp}} - m_{\text{theory}})/m_{\text{theory}}$; ^b Y indicates identification by MS/MS; ^c Denotes the relative change in BACE1 inhibited cells compared to untreated cells. NB: this is a label free determination using the peak area ratios from LC-MS/MS analyses. An up or down arrow denotes a relative change of at least 3 times, while a right arrow indicates a relative change of less than 3 times.