



C

Theoretical mass (m/z)	Experimental mass (m/z)	Charge	Error (ppm)	Sequence	Comments
817,432	817,399	+1	-40	RTNANFL	
687,321	687,309	+1	-17	RTNANF-NH ₃	ammonia lost
677,386	677,339	+1	-69	NFL-PEG2-R	
643,320	643,345	+1	39	TNANFL-H ₂ O	water lost
599,351	599,303	+1	-80	LIDRT	
557,279	557,260	+1	-34	RTNAN	
541,237	541,223	+1	-26	DRTNA-NH ₃	ammonia lost
540,253	540,233	+1	-37	DRTNA-H ₂ O	water lost
540,253	540,233	+1	-37	RTNAN-NH ₃	ammonia lost
539,269	539,254	+1	-28	RTNAN-H ₂ O	water lost
530,366	530,366	+1	0	PEG2-RLI	
530,236	530,255	+1	36	TNANF-H ₂ O	water lost
469,205	469,231	+1	55	IDRT-NH ₃	ammonia lost
468,257	468,242	+1	-32	IDRT-H ₂ O	water lost
443,236	443,220	+1	-36	RTNA	
426,210	426,196	+1	-33	RTNA-NH ₃	ammonia lost
425,226	425,216	+1	-24	RTNA-H ₂ O	water lost
398,224	398,220	+1	-10	L-PEG2-R	
384,151	384,155	+1	10	TNAN-NH ₃	ammonia lost
383,167	383,188	+1	55	TNAN-H ₂ O	water lost
373,183	373,217	+1	91	DRT	
372,199	372,187	+1	-32	RTN	
356,157	356,177	+1	56	DRT-NH ₃	ammonia lost
355,172	355,173	+1	3	DRT-H ₂ O	water lost
354,188	354,189	+1	3	RTN-H ₂ O	water lost
287,135	287,135	+1	0	TNA	
283,104	283,109	+1	18	NAN-NH ₃	ammonia lost
270,108	270,126	+1	67	TNA-NH ₃	ammonia lost
269,124	269,128	+1	15	TNA-H ₂ O	water lost
259,158	259,137	+1	-81	L-PEG2	
258,156	258,146	+1	-39	DR-H ₂ O	water lost
254,125	254,131	+1	24	RT-NH ₃	ammonia lost
241,130	241,121	+1	-37	RT-H ₂ O	water lost
240,146	240,126	+1	-83	RT	

Supplementary Figure S3. Mass spectrometry analysis of PDGF2-HTT peptide: (A) ESI chromatogram of detected ions, (B) theoretical fragments of PDGF2-HTT generated by CID, ions "b" and "y" are not marked for clarity, and (C) fragments detected during the MS/MS experiment, ions "b" and "y" are not marked for clarity. Identification of PDGF2-HTT was performed using tandem Shimadzu LC-MS IT-TOF. Pure peptide was loaded on column packed with Kromasil C8, 100 Å, 5 μm 250 × 1.0 mm and separated by linear gradient using 0.2% formic acid in water as starting and 100% acetonitrile as ending solvent (0.08 mL/min). Following MS² analysis, b and y ions of peptide were detected. The following experimental parameters were used: ion spray voltage was set at 1.7 kV, nebulizing gas flow at 1.5 L/min, and an interface heater temperature setting of 200°C. MS/MS switch criteria included precursor ions according to peptide. Data were analyzed with Shimadzu LCMS solution v3.8 software. A cutoff of 10% of intensity was applied, and the filtered data set was further analyzed manually. The following protein search parameters were used: MS tolerance 10 ppm, MS/MS tolerance 100 ppm, charge state +2–5. HTT, head-to-tail cyclization methodology.