

How Glycosaminoglycans Promote Fibrillation of Salmon Calcitonin

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Supplemental tables are related to the PRM-MS analysis and include: Table S1 Inclusion list for MS PRM-MS, Table S2 Search Parameters for PRM-MS and Table S3 Coverage Overview for PRM-MS Search

Table S1 Inclusion list

PRM-MS inclusion list for calcitonin	
Precursor ion	Sequence
619.7970	C[CAM]SNLSTC[CAM]VLGK
427.7402	LSQELHK.+2y2
746.3812	LQTYPRNTGSGTP[Ami]
389.2163	LQTYPR.+2y1
367.1774	TNTGSGTP[Ami]

Table S2 Search Parameters for PRM-MS

Search Parameters	MDM v. 1.3.0
<u>Subsamples: 2015-09-23 ETP Kirsten PRM A1.mgf, 2015-09-23 ETP Kirsten PRM B1.mgf, 2015-09-23 ETP Kirsten PRM E1.mgf</u>	
Database:	Proteins
Fasta Version:	Proteins_2015-09-22.fasta
# Sequences:	267
Taxonomy:	All entries
Enzyme:	Trypsin
Fixed modifications:	Carbamidomethyl (C)
Variable modifications:	Amidated (C-term),Oxidation (M)
Mass values:	Monoisotopic
Peptide mass tolerance:	10 ppm
Fragment mass tolerance:	0.2 Da
Max missed cleavages:	1
Instrument type:	ESI-QUAD-TOF
Ions score or expect cut-off:	0.005
Scoring :	MudPIT
<u>Subsamples: 2015-09-23 ETP Kirsten PRM A3.mgf, 2015-09-23 ETP Kirsten PRM B3.mgf, 2015-09-23 ETP Kirsten PRM E3.mgf</u>	
Database:	Proteins
Fasta Version:	Proteins_2015-09-22.fasta
# Sequences:	267
Taxonomy:	All entries
Enzyme:	Lys-C
Fixed modifications:	Carbamidomethyl (C)
Variable modifications:	Amidated (C-term),Oxidation (M)
Mass values:	Monoisotopic
Peptide mass tolerance:	10 ppm
Fragment mass tolerance:	0.2 Da
Max missed cleavages:	1
Instrument type:	ESI-QUAD-TOF
Ions score or expect cut-off:	0.005
Scoring :	MudPIT

Table S3 Coverage Overview for PRM-MS Search

2015-09-23 - PRM-MS analysis - search results														
Sample Name	Accession Nr	Protein Name	Mass kDa	Protein Sequence	Coverage %	Protein Score	Significant Matches	Unique Peptides	Peptide Score	Start	End	Duplicates	Peptide Sequences	Modifications
sCT fibrils	P01263_Pep	Calcitonin-1 Peptide 83-114	3.547	CSNLSTCVLGKLSQELHKLQ TYPRTNTGSGTP	75	1619	98	3	70	1	11	10	- .CSNLSTCVL GK.L	
Lower band									40	12	18	22	K.LSQELHK. L	
(2015-09-23 ETP Kirsten PRM A1.mgf)									58	19	24	66	K.LQTYPR.T	
sCT fibrils	P01263_Pep	Calcitonin-1 Peptide 83-114	3.547	CSNLSTCVLGKLSQELHKLQ TYPRTNTGSGTP	100	440	35	3	55	1	11	6	- .CSNLSTCVL GK.L	
Upper band									42	12	18	17	K.LSQELHK. L	
(2015-09-23 ETP Kirsten PRM A3.mgf)									42	19	32	12	K.LQTYPRTN TGSGTP.-	Amidated (C-term)
sCT fibrils added 100 weight heparin	P01263_Pep	Calcitonin-1 Peptide 83-114	3.547	CSNLSTCVLGKLSQELHKLQ TYPRTNTGSGTP	75	2087	132	3	74	1	11	10	- .CSNLSTCVL GK.L	
Lower band									41	12	18	27	K.LSQELHK. L	
(2015-09-23 ETP Kirsten PRM B1.mgf)									50	19	24	95	K.LQTYPR.T	
sCT fibrils added 100 weight heparin	P01263_Pep	Calcitonin-1 Peptide 83-114	3.547	CSNLSTCVLGKLSQELHKLQ TYPRTNTGSGTP	100	797	52	3	79	1	11	11	- .CSNLSTCVL GK.L	
Upper band									39	12	18	28	K.LSQELHK. L	
(2015-09-23 ETP Kirsten PRM B3.mgf)									29	19	32	13	K.LQTYPRTN TGSGTP.-	Amidated (C-term)
sCTHep fibrils 100%	P01263_Pep	Calcitonin-1 Peptide 83-114	3.547	CSNLSTCVLGKLSQELHKLQ TYPRTNTGSGTP	75	2471	138	3	79	1	11	18	- .CSNLSTCVL GK.L	
Lower band									37	12	18	25	K.LSQELHK. L	
(2015-09-23 ETP Kirsten PRM E1.mgf)									53	19	24	95	K.LQTYPR.T	
sCTHep fibrils 100%	P01263_Pep	Calcitonin-1 Peptide 83-114	3.547	CSNLSTCVLGKLSQELHKLQ TYPRTNTGSGTP	100	877	49	3	73	1	11	13	- .CSNLSTCVL GK.L	
Upper band									38	12	18	26	K.LSQELHK. L	
(2015-09-23 ETP Kirsten PRM E3.mgf)									29	19	32	10	K.LQTYPRTN TGSGTP.-	Amidated (C-term)