

Supplementary Table S1

TG2 peptides containing lysine residues identified as isopeptide crosslinking sites

Lysine No.	Sequence of TG2 peptide	Formula of the modification in MaxQuant and Skyline ^a	Modification mass
173	QEYVLTQQGFIYQGSAKFI	C ₁₁₀ H ₁₆₃ N ₂₅ O ₃₁	2330.19
205	FLKNAGR	C ₃₆ H ₅₇ N ₁₁ O ₉	787.43
265	WKNHGCQR	C ₄₃ H ₆₂ N ₁₆ O ₁₁ S	1010.45
380	AIKEGDLSTK	C ₄₅ H ₇₇ N ₁₁ O ₁₇	1043.55
425	SLIVGLKISTK	C ₅₃ H ₉₆ N ₁₂ O ₁₅	1140.71
429	ISTKSVGR	C ₃₅ H ₆₃ N ₁₁ O ₁₂	829.47
429	ISTKSVGRDER	C ₅₀ H ₈₇ N ₁₇ O ₁₉	1229.64
444	EDITHTYKYPEGSSSEER	C ₈₇ H ₁₂₆ N ₂₂ O ₃₄	2022.88
444	DEREDITHTYKYPEGSSSEE	C ₁₀₂ H ₁₅₀ N ₂₈ O ₄₁	2423.05
464	ANHLNKLAEKEETGMAM	C ₈₄ H ₁₄₀ N ₂₆ O ₂₈ S ₂	2024.98
464	ANHLNKLAEK	C ₄₉ H ₈₁ N ₁₅ O ₁₅	1119.60
468	LAEKEETGMAMR	C ₅₅ H ₉₃ N ₁₅ O ₂₀ S ₂	1347.62
550	SVPLCILYEKYR	C ₆₈ H ₁₀₇ N ₁₅ O ₁₈ S	1453.76
562	DCLTESNLIKVR	C ₅₈ H ₁₀₀ N ₁₆ O ₂₀ S	1372.70
562	YRDCLTESNLIKVR	C ₇₃ H ₁₂₁ N ₂₁ O ₂₃ S	1691.87
590	DLYLENPEIKIR	C ₆₈ H ₁₀₈ N ₁₆ O ₂₁	1484.79
598	ILGEPKQK	C ₄₁ H ₇₀ N ₁₀ O ₁₂	894.52
598	ILGEPKQKR	C ₄₇ H ₈₂ N ₁₄ O ₁₃	1050.62
600	QKR	C ₁₇ H ₃₁ N ₇ O ₅	413.24
600	QKRK	C ₂₃ H ₄₃ N ₉ O ₆	541.33
602	K	C ₆ H ₁₁ N ₁ O ₂	129.08
649	TVEIPDPVEAGEEVKVR	C ₈₁ H ₁₃₂ N ₂₀ O ₂₉	1848.94
663	MDLLPLHMGLHKLNVNF	C ₁₂₂ H ₁₉₈ N ₃₀ O ₃₂ S ₂	2659.42
672	LVVNFESDKLK	C ₅₉ H ₉₅ N ₁₃ O ₁₈	1273.69
672/ 674	LVVNFESDKLKAVK	C ₇₃ H ₁₂₁ N ₁₇ O ₂₁	1571.89
677	AVKGFR	C ₃₁ H ₄₉ N ₉ O ₇	659.38
Glutamine No.	Sequence of PepQ	Formula of the modification in MaxQuant and Skyline ^a	Modification mass
6	PFPQPQLPY-NH ₂	C ₅₄ H ₇₃ N ₁₁ O ₁₂	1067.54

^aFormula of TG2 peptide with NH₃ subtracted to account for the isopeptide bond