

Table 3S. Recombinant SUMO 1 fragment ion sequence assignments.Fragment **VIGQDSSEIHF**K measured as 680.63 (2+)

Measured m/z	Theoretical m/z	Ion name
213.13	213.16	b₂
270.16	270.18	b₃
294.20	294.18	y₂
398.21	398.24	b₄
431.26	431.24	y₃
513.26	513.27	b₅
544.36	544.32	y₄
600.33	600.30	b₆
760.44	760.40	y₆
816.36	816.37	b₈
847.43	847.43	y₇
929.38	929.46	b₉
962.46	962.46	y₈
1066.52	1066.52	b₁₀
1090.50	1090.52	y₉
1147.54	1147.54	y₁₀
1213.53	1213.58	b₁₁
1260.57	1260.62	y₁₁

Δm between y-n and yn-1	Fragment Ion	Measured m/z	Sequence	Measured m/z	Fragment Ion	Δm between b-n and bn-1
			Val			
113.03	1260.57	y₁₁	Ile	213.13	b₂	
57.04	1147.54	y₁₀	Gly	270.16	b₃	57.03
128.04	1090.50	y₉	Gln	398.21	b₄	128.05
115.03	962.46	y₈	Asp	513.26	b₅	115.05
86.99	847.43	y₇	Ser	600.33	b₆	87.07
216.08 (87+129)	760.44	y₆	Ser			
			Glu	816.36	b₈	216.03 (129+87)
113.10	544.36	y₄	Ile	929.38	b₉	113.02
137.06	431.26	y₃	His	1066.52	b₁₀	137.14
	294.20	y₂	Phe	1213.53	b₁₁	146.99
			Lys			