

Table 1S. Ubiquitin Fragment Ion Sequence Assignments.

Fragment TITLEVEPSDTIENVK measured as 894.80 (2+)

Measured m/z	Theoretical m/z	Ion name
360.30	360.22	y-3
429.26	429.27	b-4
489.33	489.27	y-4
558.36	558.31	b-5
602.55	602.35	y-5
657.34	657.38	b-6
703.48	703.40	y-6
786.43	786.42	b-7
818.44	818.43	y-7
970.50	970.51	b-9
1002.52	1002.51	y-9
1131.55	1131.55	y-10
1230.62	1230.62	y-11
1299.57	1299.67	b-12
1359.67	1359.66	y-12
1428.55	1428.71	b-13
1472.79	1472.75	y-13
1542.68	1542.75	b-14
1573.67	1573.80	y-14
1641.78	1641.82	b-15

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
			Thr			
			Ile			
100.88	y-14	1573.67	Thr			
113.12	y-13	1472.79	Leu	429.26	b-4	
129.05	y-12	1359.67	Glu	558.36	b-5	129.10
99.05	y-11	1230.62	Val	657.34	b-6	98.98
129.07	y-10	1131.55	Glu	786.43	b-7	129.09
184.08 (97+87)	y-9	1002.52	Pro			
			Ser	970.50	b-9	184.07 (97+87)
114.96	y-7	818.44	Asp			
100.93	y-6	703.48	Thr			
113.22	y-5	602.55	Ile	1299.57	b-12	
129.03	y-4	489.33	Glu	1428.55	b-13	128.98
	y-3	360.30	Asn	1542.68	b-14	114.13
			Val	1641.78	b-15	99.10
			Lys			