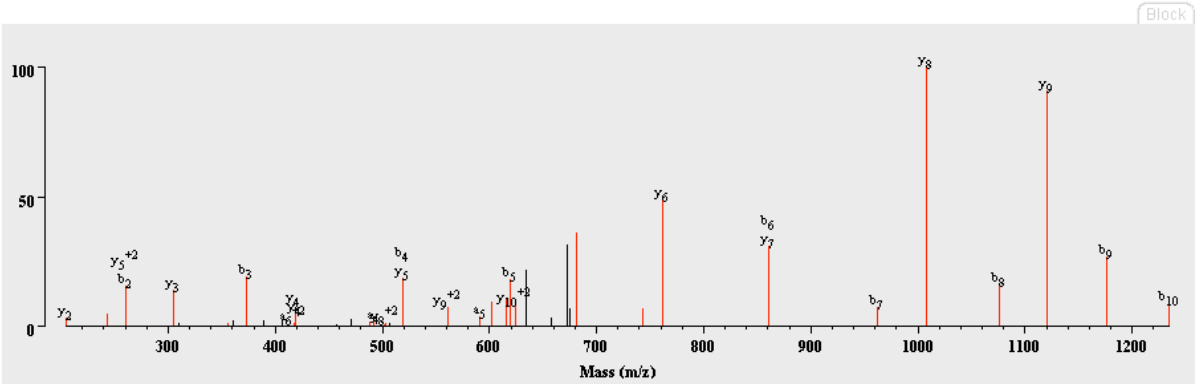
Supplementary figure 1
Ubiquitin chain linkages

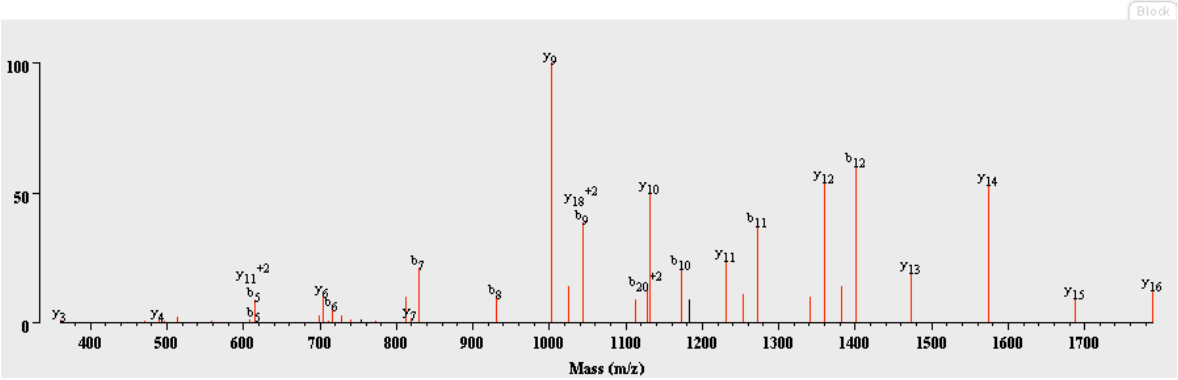
Ubiquitin K6 m/z 690.39 MQIFVK(GlyGly)TLTGK^{+2}



m/z	Ion Type
204.219	y2
243.083	y5-2H2O+2
260.055	b2
305.266	y3
356.272	b3-NH3
373.196	y6-H2O+2
417.849	a6+2
418.45	y4
488.263	y8-2NH3+2
491.438	a4
501.191	y5-H2O
503.492	b4-NH3
519.302	y5
560.973	y9+2
591.297	y10-H2O-3NH3+2
602.274	b5-NH3
616.055	y10-H2O+2
619.235	b5
624.891	y10+2
681.576	MH-H2O+2
743.624	y6-H2O
761.428	y6
860.556	y7
962.372	b7
1007.62	y8
1075.73	b8
1120.71	y9
1176.61	b9
1233.72	b10

Ubiquitin K11 m/z 1201.64

TLTGK(GlyGly)TITLEVEPSDTIENVK^{+2}

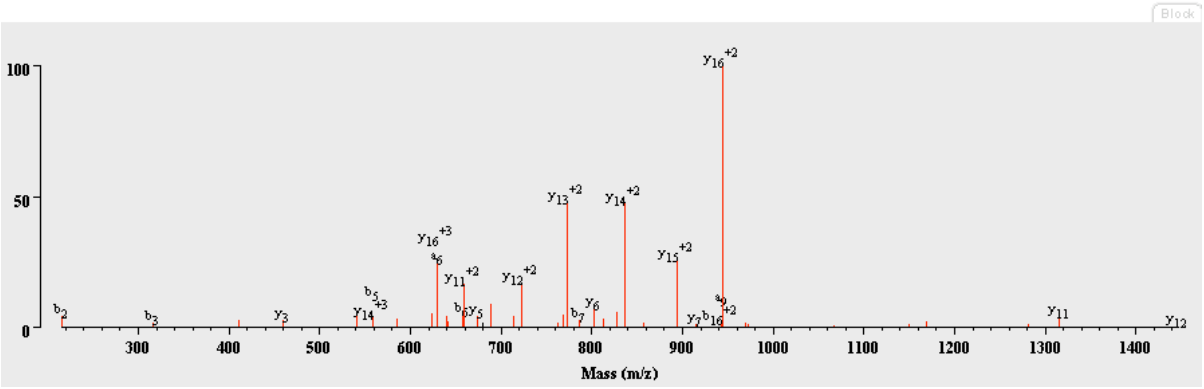


m/z	Ion Type
360.029	y3
471.245	y4-H2O
489.316	y4
496.576	b9-2H2O-NH3+2
514.329	b9-NH3+2
558.437	y10-NH3+2
607.308	y11-H2O+2
614.796	b5
615.512	b5
698.369	b6-H2O
703.41	y6
710.372	y13-3H2O+2
716.425	y14-7H2O-NH3+2
728.586	y13-H2O+2
740.484	b13-H2O+2
773.63	y15-6H2O-2NH3+2
811.444	b16-9H2O-NH3+2
818.428	y15-H2O-2NH3+2
829.441	b16-8H2O+2
930.497	y9-4H2O
1002.45	y9
1025.5	b19-6H2O+2
1043.45	y10-4H2O-NH3
1113.52	y10-H2O
1128.74	b20+2
1131.54	y10
1172.56	b10
1230.53	y11
1253.56	y12-5H2O-NH3
1271.65	y12-3H2O-2NH3
1341.6	y12-H2O
1359.67	y12
1382.67	y13-5H2O

1400.72	y13-4H2O
1472.67	y13
1573.81	y14
1686.87	y15
1788.06	y16

Ubiquitin K27 m/z 701.04

TITLEVEPSDTIENVK(GlyGly)AK^{+3}

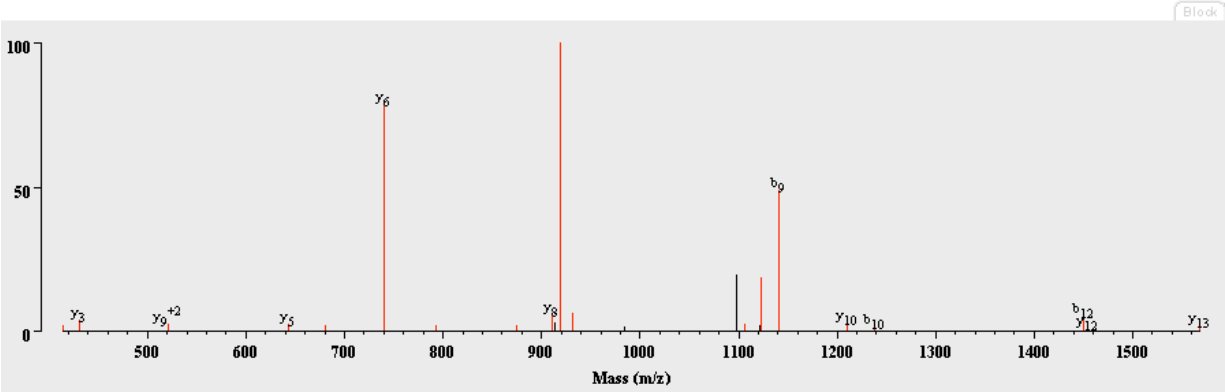


m/z	Ion Type
214.986	b2
316.11	y8-2H2O-2NH3+3
411.216	b4-H2O
460.258	y3
540.131	y9-3H2O+2
558.133	y10-3H2O-3NH3+2
584.991	y10-3NH3+2
623.766	y11-3H2O-NH3+2
629.778	a6
639.252	y17-2H2O-3NH3+3
641.441	y11-H2O-NH3+2
657.087	y5-NH3
658.645	y11+2
673.294	y5
689.28	y12-H2O-3NH3+2
713.809	y12-H2O+2
723.021	y12+2
763.175	y13-H2O+2
768.351	y6-H2O-NH3
772.54	y13+2
786.106	y6-NH3
802.343	y14-3H2O-NH3+2
812.345	y14-3NH3+2

827.213	y14-H2O+2
828.071	y14-H2O+2
837.04	y14+2
857.776	y15-4H2O+2
893.623	y15+2
915.153	b17-7H2O+2
942.669	b17-4H2O+2
943.799	b17-2H2O-2NH3+2
969.129	b17-H2O+2
973.048	y17-3H2O+2
1067.32	b10-H2O
1150.35	y10-H2O-3NH3
1168.39	y10-3NH3
1281.51	y11-H2O-NH3
1315.45	y11
1444.62	y12

Ubiquitin K29 m/z 940.49

AK(GlyGly)IQDK(Carbamyl)EGIPPDQQR^{+2}

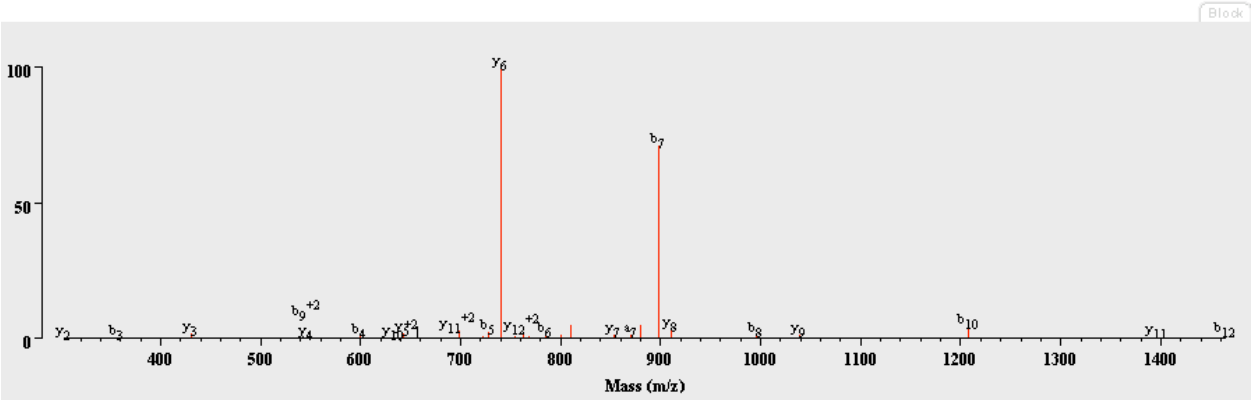


m/z	Ion Type
413.749	y3-NH3
431.423	y3
520.591	y9+2
643.523	y5
680.591	b12-3H2O-2NH3+2
740.48	y13-3H2O-2NH3+2
792.681	b14-3H2O-4NH3+2
875.061	y8-H2O-NH3
910.072	y8
919.154	b7-H2O-2NH3
931.753	MH-H2O+2

1105.56	b9-2H2O
1123.3	b9-H2O
1140.52	y10-2H2O-2NH3
1210.81	y10
1237.68	y11-3H2O-2NH3
1449.82	b12
1454.08	y12
1567.19	b14-3H2O-5NH3

Ubiquitin K33 m/z 819.42

IQDK(GlyGly)EGIPPDQQR^{+2}

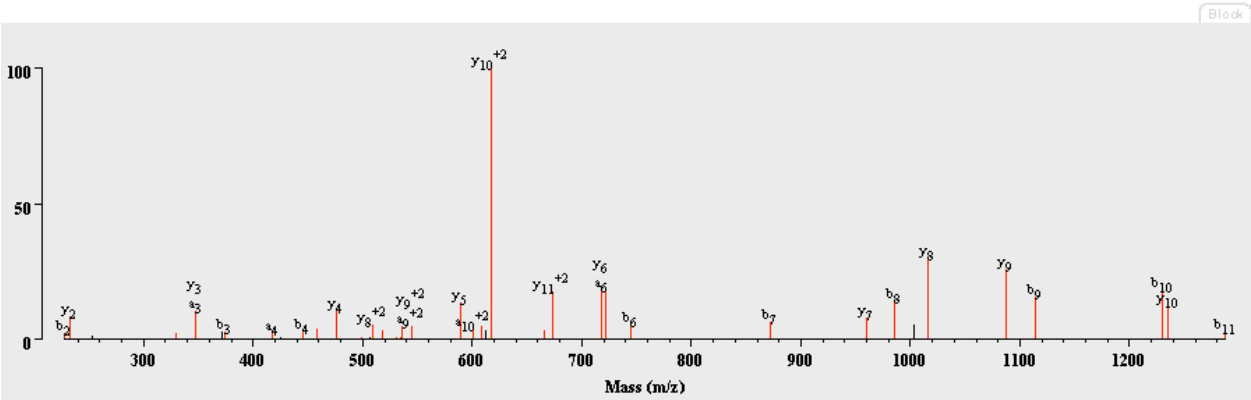


m/z	Ion Type
303.201	y2
312.343	y5-H2O+2
340.023	b3-H2O
357.101	b5-NH3+2
396.332	y3-2NH3
413.265	y3-NH3
430.217	y8-H2O-2NH3+2
431.349	y3
546.304	y4
599.258	y10-H2O-4NH3+2
615.278	y10-2H2O-NH3+2
637.166	y11-3H2O-4NH3+2
638.136	y11-3H2O-4NH3+2
641.388	b11-3H2O+2
643.252	b11-H2O-2NH3+2
699.099	b12-4NH3+2
722.202	y6-H2O
728.145	y12-3H2O-NH3+2

740.306	y6
754.122	y12-H2O+2
762.502	y12+2
768.286	b6-H2O
785.198	y7-H2O-3NH3
801.123	y7-H2O-2NH3
810.634	MH-H2O+2
853.451	y7
870.191	a7
880.261	b7-H2O
898.313	b7
910.32	y8
995.561	b8
1039.44	y9
1207.38	b10
1396.67	y11
1463.63	b12

Ubiquitin K48 m/z 730.90

LIFAGK(GlyGly)QLEDGR^{+2}

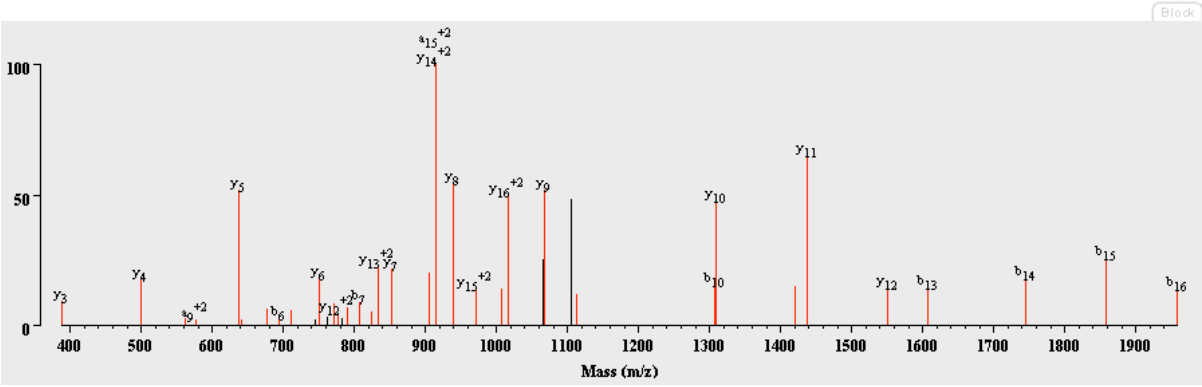


m/z	Ion Type
227.035	b2
232.226	y2
329.056	y3-H2O
347.192	a3
374.198	b3
417.162	a4
445.293	y7-2H2O-2NH3+2
458.313	y4-H2O
476.285	y4
499.484	y8-H2O+2

508.673	y8+2
518.29	y9-2H2O-NH3+2
531.38	b9-H2O-2NH3+2
534.387	y9-H2O+2
535.993	y9-H2O+2
544.344	a9+2
589.417	b10-2H2O-NH3+2
600.492	y10-2H2O+2
609.089	b11-2H2O-2NH3+2
617.962	b11-2H2O-NH3+2
665.391	y6-H2O-2NH3
673.894	y11+2
717.395	a6
721.878	MH-H2O+2
744.533	b6
872.575	y7-2H2O-3NH3
959.684	y7
985.611	b8
1016.61	y8
1087.7	y9
1114.63	b9
1229.66	b10
1234.81	b11-H2O-2NH3
1286.62	b11

Ubiquitin K63 m/z 1122.61

TLSDYNIQK(GlyGly)ESTLHLVLR^{+2}



m/z	Ion Type
387.379	y3
500.362	y4
561.941	b5-H2O

576.267	a9+2
637.517	b10-2NH3+2
641.302	b6-2H2O-NH3
676.146	y11-3H2O-2NH3+2
694.089	y11-H2O-2NH3+2
710.629	y11-H2O+2
750.583	y12-H2O-2NH3+2
771.3	b7-2H2O
772.256	b7-2H2O
776.221	y12+2
789.397	y13-3H2O-2NH3+2
807.382	y13-2H2O-NH3+2
824.674	y13-H2O+2
833.172	y13+2
851.562	y7
906.153	y14-H2O+2
914.793	y14+2
938.596	y15-4NH3+2
972.255	y16-3H2O-2NH3+2
1006.77	y16-H2O+2
1015.77	y16+2
1067.61	y9
1113.66	MH-H2O+2
1306.53	b11-3H2O-2NH3
1309.85	y10
1419.75	y11-H2O
1437.88	y11
1550.86	y12
1607.6	b13
1745.04	b14
1857.96	b15
1957.16	b16