

Supplementary Mass spectrometry Data 2. Summary of the identified ADP-ribosylation sites in human PARP1 protein and the representative fragmentation spectra. adpr = mono(ADP-ribosylation); ri = ribose phosphate

Position	PEP	Score	Modified Sequence	Charge	m/z	Mass Error [ppm]
Glu3	1.30E-17	152.6	_GSHHMAE(adpr)SSDK_	3	576.1903	0.9313
Glu147	2.42E-07	130.9	_MVDPE(adpr)KPQLGMIDRWYHPGCFVK_	4	836.8587	-0.8299
	1.92E-11	136.4	_MVDPE(adpr)KPQLGMIDR_	3	723.9631	0.2965
	8.41E-11	122.0	_MVDPE(adpr)K_	2	630.2062	0.4358
	3.79E-20	156.0	_MVDPE(ri)KPQLGMIDR_	3	614.2789	-0.7912
Glu168 or Glu169	6.25E-33	189.8	_E(adpr)ELGFRPEYSASQLK_	3	765.6504	2.0339
	3.81E-16	200.3	_NRE(adpr)ELGFRPEYSASQLK_	3	855.6984	0.9941
	5.80E-33	228.5	_NREE(ri)LGFRPEYSASQLK_	3	746.0142	0.4331
Glu190	1.09E-10	191.2	_GFSLLATE(adpr)DK_	2	811.3128	2.4288
	5.02E-24	165.0	_GFSLLATE(ri)DK_	2	646.7865	0.3807
Glu471	9.58E-18	221.0	_SLQE(adpr)LFLAHILSPWGAEVK_	3	893.7467	0.9412
Glu484	8.55E-53	215.5	_SLQELFLAHILSPWGAE(adpr)VK_	3	893.7467	-0.1173
Glu488	2.79E-11	123.0	_AE(ri)PVEVVAPR_	2	639.8025	0.2745
Glu491	3.25E-06	117.0	_AEPVE(adpr)VVAPRGK_	3	598.2604	0.6256
	6.47E-11	112.7	_AEPVE(ri)VVAPR_	2	639.8025	-0.0397
	1.11E-06	122.2	_AEPVE(ri)VVAPRGK_	2	732.3607	-0.2284



































