

Table S2: y_n Ions for Benzoquinone-modified and Unmodified Model Peptides

NON-TRYPTIC PEPTIDES	[M+H] ⁺	[M+2H] ²⁺	C/D m/z	y1	y2	y3	y4	y6	y7	y8	y9	y10	y11	y12	y13	y14	y15	y16	y17	y18	y19
AGAGAGAG (modified)	742.3	671.7	742.0																		
AGAGAGAG	633.3	317.1	634.0		147.0		274.9			560.4											
CYQNCPLG-NH2 (modified)	1225.5	613.3	614.0		187.8	284.9	487.9	739.9													
CYQNCPLG-NH2	1009.5	505.2	505.0		187.6	282.0	397.0	630.2	743.0												
EDVSAGDCGPLEGGPE (modified)	1865.7	933.4	933.4		244.9	303.2	359.3	1244.9	1585.6	696.0						1435.1	1522.7			1620.1	
EDVSAGDCGPLEGGPE	1757.8	879.4	879.4		301.8	359.3	469.6	585.0							1256.6	1327.4	1414.8			1514.0	
EDVSAGDCGPLEGGPE	1027.5	514.3	514.1	132.0	279.0		505.9	717.3				955.3	1070.0								
RGPCRAFI (modified)	919.1	460.1	460.0		278.0			762.5													
SSDCFGSR (modified)	967.0	484.0	966.6				466.3	677.3	792.3	878.1											
SSDCFGSR	858.3	429.7	858.5				316.6	466.5	684.5	771.3											
IGASGMGCGR (modified)	1145.3	573.2	1144.6				444.0	500.3	688.4	775.3	974.5	1031.7									
IGASGMGCGR	1036.5	518.7	1036.5						580.2												
SSDCFGSRDR (modified)	1351.4	676.2	1350.7							1061.5	1176.5										
SSDCFGSRDR	1242.6	621.8	1242.7																		
AVAGCAGAR (modified)	883.4	442.2	883.4				374.2	585.3	643.4	714.6											
AVAGCAGAR	774.4	387.7	775.0			303.0	374.0		534.2	605.3											
SHCIAVEK (modified)	1123.5	562.3	1123.4			374.2		575.2	688.3	899.3	1038.4										
SLHTLFQDELCK (modified)	1470.7	735.9	1471.5				599.4	715.1	772.2	919.4	1032.3										
SLHTLFQDELCK	1362.7	681.8	1362.5																		
LCVLEK (modified)	949.5	475.2	949.4																		
GACLLPK (modified)	809.4	405.2	809.4																		
MOCTEDYLSILNAR (modified)	1775.8	888.4	1775.6																		
LFTFHADICTLPDTEK (modified)	1958.9	980.0	1958.8																		
LKPDNTLGDFAEDK (modified)	1627.8	814.4	1627.7																		
LKPDNTLGDFAEDK (modified)	2071.0	1036.0	2070.9																		
DAIPENLPLTADFAEDK (modified)	2509.2	1255.1	2509.1																		
DHFACTYSTVDFK (modified)	1605.7	803.3	1605.6																		
NEFLSHKDDSPDLPK (modified)	1952.9	976.9	1952.8																		
YICNDQITSSK (modified)	1494.6	747.8	1494.5																		
RPGFSALTDETYTPK (modified)	1931.9	966.5	1931.8																		
ECCDKPLEK (modified)	1393.6	697.3	1393.5																		
ECCDKPLEK	1177.6	589.3	1177.5																		
SHCIAVEK (modified)	1123.5	562.3	1123.4																		
TCVADESHAGCEK (modified)	1565.6	783.3	1565.5																		
IGASGMGCGR (modified)	1144.5	572.8	1144.4																		
IGASGMGCGR	1035.5	518.2	1035.4																		
SSDCFGSRDR (modified)	1351.4	676.2	1351.3																		
SSDCFGSRDR	1242.6	621.8	1242.5																		
AVAGCAGAR (modified)	883.4	442.2	883.3																		
AVAGCAGAR	774.4	387.7	774.3																		

Note: Number in [] are doubly charged ion