Protein	Peptide Sequence	Q1 m/z	Q3 m/z	Fragment Type	Predicted Intensity (GPM)	Intensity (Expt.)
ACTB	AGFAGDDAPR	560.8	630.3	y6	100	15
			701.3	y7	46	12.2
			343.2	y3	61	100
			424.7	$y8^{2+}$	33	0
			420.2	b3	16	21. 7
	GYSFTTTAER	638.9	581.3	$b4-H_2O$	20	35.1
			452.2	b3	37	72.2
			678.3	y6	100	82.8
			912.4	y8	77	100
			577.3	y5	50	50.3
	SYELPDGQVITIGNER	968.0	1086.6	y10	13	37.3
			706.4	$y13^{2+}$	30	1.1
			1298.7	y12	100	100

Peptide		m/z	Ion		
		475.2	y4	65	28.2
		689.4	y6	62	23.3
HQGVMVGMGQK	730.4	393.2	b2-NH$_3$	27	0.1
		566.3	b4	13	100
		1050.6	y9	100	0
		410.2	b2-NH$_3$	52	17.2
		664.4	y5	34	38.6
TVLSGGTTMYPGIADR	892.0	628.3	y6	100	28.5
		1155.6	b10	37	1.9
		791.4	y7	37	3.1
		345.2	b2	37	100
		1023.5	y9	17	24.4
TGIVMDSGDGVTH	767.4	918.4	y9	64	6.7
		499.3	b4-H$_2$O	20	30.6
		1017.4	y10	53	9.8

			386.2	b3-H_2O	100	100
			87.3	y8	38	21.9
THBS1	GFLLLASLR	567.3	672.4	y6	41	24.5
			462.3	b3	18	100
			446.3	y4	100	25.3
			559.4	y5	81	8.6
			688.4	b5	77	6.7
	FVFGTTPEDILR	769.9	742.4	y6	100	100
			574.8	y10^{2+}	79	0
			363.2	a2	87	16.7
			688.9	y12-H_2O^{2+}	50	0
			565.8	y10-H_2O^{2+}	56	1.2
	GGVNDNFQGVLQNVR	880.9	1083.5	b11-H_2O	12	8.3

	871.4	b9-H_2O	12	6.2
	629.4	y5	100	85.4
	913.5	y8	47	35.4
	785.5	y7	62	100
IPESGGDNSVFDIFELTGAAR	1170.1	864.5 y8	62	40.3
	1092.6	y10	48	15.1
	1239.6	y11	100	64.3
	1041.5	y20^{2+}	73	0
	977.5	y9	56	100
SITLFVQEDR	676.4	504.3 y8^{2+}	23	1.7
	397.2	y6^{2+}	20	21.4
	595.3	y18-$H_2O$$^{2+}$	100	2.7

		793.4	y6	58	100
		646.3	y5	46	24.4
DCVGDVTENQICNK	908.9	909.4	y6	81	7.6
		554.2	y3	50	100
		1130.5	y8	100	7.3
		1410.6	y11	38	1.6
		779.3	b6	38	18

Supplemental Table 2: A comparison of GPM-predicted fragment ion intensities and experimentally-determined fragment ion intensities from peptides labeled with iTRAQ. Table 1 lists GPM-predicted MRM transitions for several peptides from β-Actin (ACTB, swissprot accession number P60709) and Thrombospondin-1 (THBS1, swissprot accession number P07996), and compares fragment ion intensity values predicted by the GPM vs experimentally determined intensity values.