Supplemental Information

Cross-Linking Evidence for Multiple Interactions of the PsbP and PsbQ Proteins in a Higher Plant Photosystem II Supercomplex

Kunio Ido[a], Jon Nield[b], Yoichiro Fukao[c], Fumihiko Sato[a], and Kentaro Ifuku[a,d,]

[a]Graduate School of Biostudies, Kyoto University, Sakyo-ku, Kyoto 606-8502, Japan; [b]School of Biological and Chemical Sciences, Queen Mary University of London, London E1 4NS, United Kingdom; [c]Plant Global Educational Project, Nara Institute of Science and Technology, Ikoma, 630-0192 Japan; [d]Japan Science and Technology Agency, PRESTO, 4-1-8 Honcho Kawaguchi, Saitama 332-0012, Japan

Table S1: Peptide list for the band P-1 identified by the LC-MS analysis.
Table S2: Peptide list for the band P-2 identified by the LC-MS analysis.
Table S3: Peptide list for the band P-3 identified by the LC-MS analysis.
Table S4: Peptide list for the band P-4 identified by the LC-MS analysis.
Table S5: Peptide list for the band Q-3 identified by the LC-MS analysis.
Table S6: Peptide list for the band Q-4 identified by the LC-MS analysis.

Table S7: The lists of detected product ions derived from peptides that were predicted to be cross-linked between PsbP and PsbR.

Table S8: The lists of detected product ions derived from peptides that were predicted to be cross-linked between PsbP and CP26.

Table S1: Peptide list for the band P−1 identifided by the LC−MS analysis

Index	scan#	charge	score	pp	pp2	pp_tag	RT_conf	RT(obs)	RT(pred)	PA	m/z	MW(obs)	MW	delta	miss	peptide+modif	protein
1483	1047	2	88	19.6	13.8	18.2	0.6746	17.13	18.11	178832.06	740.8597	1480.7122	1480.7101	0.0022	0	SPTGEVIFGGETMR	CP43
1488	930	2	71	16.1	12.4	10.7	0.3711	15.46	18.11	12356.65	748.8571	1496.7068	1496.705	0.0019	0	SPTGEVIFGGETMR OxiM(13)	CP43
1446	754	2	51	24.3	10.2	13.6	0.9866	12.3	12.35	1235223.9	713.887	1426.7666	1426.7649	0.0018	0	LGANVGSAQGPTGLGK	CP43
953	389	1	38	10	18.8	5.5	0.3931	7.02	10.39	11763.57	764.3934	764.3934	764.3937	−0.0003	0	AAAAGFEK	CP43
954	422	1	33	10.8	16.9	5.5	0.3931	7.02	10.39	11763.57	764.3945	764.3945	764.3937	0.0007	0	AAAAGFEK	CP43
1573	1238	2	89	16.1	11.1	10.3	0.4356	20.11	23.55	848704.73	910.449	1819.8908	1819.8895	0.0013	1	GIDRDFEPVLSMTPLN OxiM(12)	CP43
1072	1164	2	82	11.6	15.7	9.1	0.6592	18.89	17.87	228372.02	491.2798	981.5523	981.5516	0.0007	0	APWLEPLR	CP43
1163	774	2	26	18.4	6.6	9.9	0.7384	12.62	13.42	494264.82	536.2648	1071.5224	1071.5218	0.0006	0	DIQPWQER	CP43
938	770	1	50	12.2	21	4.6	0.8747	12.65	13.03	94794.62	744.4631	744.4631	744.4614	0.0017	0	LINLSGK	CP43
1289	676	2	23	11.8	7.1	4.9	0.4588	10.98	13.11	9913.74	614.3154	1227.6235	1227.6229	0.0006	1	DIQPWQERR	CP43
59	1666	1	58	7.9	14.2	2.1	0.0966	26.88	8.88	67207.23	460.2545	460.2545	460.2514	0.0031	0	GIDR	CP43
930	1060	1	31	6.2	11.1	2.3	0.4765	17.27	15.5	200745.72	736.3788	736.3788	736.3777	0.0011	0	FWDLR	CP43
1596	1296	3	37	3.9	6.3	5.8	0.5668	20.99	23.19	369505.47	631.3396	1892.0042	1892.0219	−0.0176	1	*APWLEPLRGPNGLDLSR	CP43

Table S2: Peptide list for the band P-2 identifided by the LC-MS analysis

Index	scan#	charge	score	pp	pp2	pp_tag	RT_conf	RT(obs)	RT(pred)	PA	m/z	MW(obs)	MW	delta	miss	peptide+modif	protein
1062	741	2	143	21.5	20.3	10.1	0.5185	12.26	12.95	447952.02	485.7641	970.5209	970.5204	0.0005	0	DPDQAALLK	CP26
1063	743	1	33	15.1	9.8	7.3	0.5193	12.26	12.95	109155.25	970.5219	970.5219	970.5204	0.0015	0	DPDQAALLK	CP26
1427	1191	2	33	9.8	6.2	9.1	0.518	19.62	18.89	70567.57	709.8929	1418.7785	1418.7791	−0.0006	0	LHPGGPFDPLGLAK	CP26
1428	1193	3	54	10.4	11.2	15.3	0.5396	19.58	18.89	229904.81	473.5984	1418.7807	1418.7791	0.0016	0	LHPGGPFDPLGLAK	CP26
1472	1181	2	89	19.9	16.1	11.8	0.4813	19.44	18.64	193796.92	741.8465	1482.6857	1482.6834	0.0023	0	FGANCGPEAVWFK	CP26
1313	997	2	54	16.7	11.5	11.2	0.3144	16.46	17.62	1391716	624.3302	1247.6531	1247.6531	0	0	YQAFELIHAR	CP26
1577	1265	2	37	10.9	8	15.8	0.0138	20.75	25.98	118436.63	925.9523	1850.8973	1850.8928	0.0045	0	WAMLGAAGCVIPEAFNK OxiM(3)	CP26
723	269	1	67	12.4	16.2	3.7	0.6648	4.91	4.4	20464.54	616.4026	616.4026	616.4028	−0.0002	1	VKEIK	CP26
724	300	1	64	13	16.5	3.7	0.6648	4.91	4.4	20464.54	616.4036	616.4036	616.4028	0.0008	1	VKEIK	CP26
986	329	1	59	13.7	14.7	4.2	0.8887	5.46	5.62	53169.74	834.4376	834.4376	834.4356	0.002	1	KPEDFAK	CP26
1524	1313	2	40	14.1	7.9	7.1	0.0088	21.52	27.84	39241.89	848.9509	1696.8945	1696.8905	0.004	0	TGALLLDGNTLNYFGK	CP26
723	269	1	40	9.6	13.1	3.7	0.4877	4.91	4.06	20464.54	616.4026	616.4026	616.4028	−0.0002	1	IEKVK	N/A
1669	1271	3	30	10.7	3.8	6.3	0.0115	20.82	26.42	105744.81	790.7662	2370.284	2370.2816	0.0024	1	LHPGGPFDPLGLAKDPDQAALLK	CP26

Table S3: Peptide list for the band P-3 identifided by the LC-MS analysis

Index	scan#	charge	score	pp	pp2	pp_tag	RT_conf	RT(obs)	RT(pred)	PA	m/z	MW(obs)	MW	delta	miss	peptide+modif	protein
1185	320	2	59	20.8	10.5	8.7	0	4.89	0	122623.51	531.2708	1061.5343	1061.5334	0.0009	1	LRDGVDSSGR	PsbR
1186	289	2	47	10.9	10.5	3.6	0	4.8	0	275617.58	531.2718	1061.5363	1061.5334	0.0029	1	LRDGVDSSGR	PsbR
1187	297	1	19	18.3	5.8	5.2	0	5	0	5088.55	1061.5372	1061.5372	1061.5334	0.0038	1	LRDGVDSSGR	PsbR
1095	842	2	74	17.7	11.3	7.3	0	13.92	0	29584.61	478.2484	955.4895	955.4884	0.0012	0	GVYQFVDK	PsbR
1096	844	1	34	11.4	16.8	4.8	0	13.85	0	8046.28	955.4903	955.4903	955.4884	0.0019	0	GVYQFVDK	PsbR
1470	731	3	32	12.2	5.4	16.1	0	12.17	0	20967.73	476.9469	1428.8261	1428.8243	0.0018	2	IKVDKPLGIGGGMK OxiM(13)	PsbR
1302	616	2	39	18.5	6.2	8.2	0	9.86	0	357613.82	594.327	1187.6468	1187.6453	0.0015	1	VDKPLGIGGGMK OxiM(11)	PsbR
1405	247	2	41	10.8	8.9	6.2	0	4.02	0	5405	652.3341	1303.6609	1303.6601	0.0009	2	DGVDSSGRKPTGK	PsbR

Table S4: Peptide list for the band P-4 identifided by the LC-MS analysis

Index	scan#	charge	score	pp	pp2	pp_tag	RT_conf	RT(obs)	RT(pred)	PA	m/z	MW(obs)	MW	delta	miss	peptide+modif	protein
1515	1189	2	139	24.5	18.3	12.4	0.6734	19.34	20.51	68839.77	743.3467	1485.6862	1485.6856	0.0006	0	FDSLEQLDEFSR	PsbE
1239	1329	2	89	11.5	15.8	14.4	0.6603	21.36	20.16	123110.61	561.8125	1122.6177	1122.6154	0.0024	0	SFADIITSIR	PsbE
1088	1065	2	65	14.2	9	9.8	0.4571	17.18	14.9	1082437.6	477.7901	954.573	954.5731	−0.0001	0	QGIPLITGR	PsbE
1089	1063	1	36	14.9	7.6	7.1	0.4502	17.23	14.9	96215.35	954.5731	954.5731	954.5731	0	0	QGIPLITGR	PsbE
1265	640	2	81	14.6	15.2	7.6	0.9887	10.4	10.44	15465.55	571.7604	1142.5136	1142.5113	0.0023	0	PNEYFTESR	PsbE

Table S5: Peptide list for the band Q−3 identifided by the LC−MS analysis

Index	scan#	charge	score	pp	pp2	pp_tag	RT_conf	RT(obs)	RT(pred)	PA	m/z	MW(obs)	MW	delta	miss	peptide+modif	protein
1303	840	3	111	15.4	14.6	16.8	0.1984	13.69	16.98	4109.76	499.5737	1496.7065	1496.705	0.0015	0	SPTGEVIFGGETMR OxiM(13)	CP43
1304	839	2	69	16	12.2	16.8	0.1851	13.44	16.98	244874	748.857	1496.7067	1496.705	0.0017	0	SPTGEVIFGGETMR OxiM(13)	CP43
1241	1179	2	58	23.4	9.4	13.2	0.3279	19.52	22.51	9807.78	689.8323	1378.6573	1378.6559	0.0014	0	DFEPVLSMTPLN OxiM(8)	CP43
1273	707	2	41	20.5	9.4	10.7	0.2975	11.6	9.71	7199.87	713.8873	1426.7673	1426.7649	0.0024	0	LGANVGSAQGPTGLGK	CP43
905	651	2	59	17.1	11.7	9.8	0.6596	10.27	10.8	57769.27	464.7458	928.4844	928.4847	−0.0003	0	GPNGLDLSR	CP43
948	1015	2	123	11.6	16.3	9.1	0.9875	16.7	16.68	12589.58	491.2798	981.5524	981.5516	0.0007	0	APWLEPLR	CP43
769	696	1	54	14	20.6	4.6	0.6741	11.07	10.57	11538.93	744.4622	744.4622	744.4614	0.0007	0	LINLSGK	CP43
1030	727	2	30	15.3	7.1	8.6	0.6833	11.54	11.06	102991.38	536.2645	1071.5217	1071.5218	−0.0001	0	DIQPWQER	CP43
791	371	1	44	7.9	17.6	4	0.5087	6.1	7.24	294.33	764.3952	764.3952	764.3937	0.0015	0	AAAAGFEK	CP43
1383	1117	2	80	9.7	10.3	6.2	0.2034	18.21	23.85	147761.65	910.4489	1819.8906	1819.8895	0.0011	1	GIDRDFEPVLSMTPLN OxiM(12)	CP43
1589	1144	3	41	9.6	6.7	7.9	0.2113	18.68	24.25	171536.04	1107.5476	3320.6283	3320.6216	0.0067	0	SAEYMTHAPLGSLNSVGGVATEINAVNYVSPR OxiM(5)	CP43

Table S6: Peptide list for the bandQ-4 identifided by the LC-MS analysis

Index	scan#	charge	score	pp	pp2	pp_tag	RT_conf	RT(obs)	RT(pred)	PA	m/z	MW(obs)	MW	delta	miss	peptide+modif	protein
1158	796	2	195	19	22.8	10.1	0.487	12.63	14.34	168644.39	485.7641	970.5209	970.5204	0.0005	0	DPDQAALLK	CP26
1159	801	1	31	14	8.9	4.8	0.4734	12.57	14.34	1816.49	970.521	970.521	970.5204	0.0006	0	DPDQAALLK	CP26
1160	832	2	12	19	5.8	10.1	0.5102	12.73	14.34	56588.05	485.765	970.5228	970.5204	0.0024	0	DPDQAALLK	CP26
1436	1177	3	66	12.8	11.5	18.5	0.4636	19.25	17.57	33085.85	473.5978	1418.779	1418.7791	−0.0001	0	LHPGGPFDPLGLAK	CP26
1437	1215	3	20	7.1	7.6	7.2	0.5941	18.76	17.57	1397492.6	473.5983	1418.7804	1418.7791	0.0014	0	LHPGGPFDPLGLAK	CP26
1438	1179	2	30	7.5	5.6	1.7	0.5372	18.96	17.57	29727.6	709.894	1418.7807	1418.7791	0.0016	0	LHPGGPFDPLGLAK	CP26
1511	1318	2	124	23.1	18	11.5	0.6393	21.15	22.43	1155430.1	848.9495	1696.8916	1696.8905	0.0012	0	TGALLLDGNTLNYFGK	CP26
1472	1186	2	102	18.5	17.3	10.7	0.4823	19.03	17.43	53228.27	741.8461	1482.6849	1482.6834	0.0014	0	FGANCGPEAVWFK	CP26
1289	889	2	75	24.2	12.1	8.1	0.8993	14.1	14.39	91890.21	576.2838	1151.5604	1151.5579	0.0025	0	ITNGLDFEDK	CP26
1544	1366	2	43	9.7	10.1	11.1	0.8118	22.02	21.42	36545.05	917.9539	1834.9004	1834.8979	0.0026	0	WAMLGAAGCVIPEAFNK	CP26
1358	1013	2	46	11.2	10.8	10	0.7755	16.25	16.88	8775.65	624.3327	1247.6581	1247.6531	0.005	0	YQAFELIHAR	CP26

Table S7: The lists of detected product ions derived from peptides that were predicted to be cross-linked between PsbP and PsbR.

Index	scan#	charge	score	pp	pp_2	pp_{tag}	m/z	MW(obs)	MW	delta	miss		Unique sequence + modifications
1998	372	+4	49	24.0	9.6	4.7	505.7815	2020.1043	2020.0934	0.0109	0	√	RD($1)GVDSSGRKPTGKGVY K($1)L

chainA :

#	$b^{\prime+4}$	b^{*+4}	b^{+4}	$b^{\prime+3}$	b^{*+3}	b^{+3}	$b^{\prime++}$	b^{*++}	b^{++}	$b^{\prime+}$	b^{*+}	b^{+}	seq	$y^{\prime+4}$	y^{*+4}	y^{+4}	$y^{\prime+3}$	y^{*+3}	y^{+3}	$y^{\prime++}$	y^{*++}	y^{++}	$y^{\prime+}$	y^{*+}	y^{+}	#
1	—	35.78	40.03	—	47.37	53.04	—	70.54	79.06	—	140.08	157.11	R	501.28	501.52	505.78	**668.03**	**668.36**	674.04	1001.55	1002.04	1010.55	2002.08	2003.07	2020.09	M
2	124.58	124.83	129.08	**165.77**	166.1	171.78	**248.16**	**248.65**	**257.16**	**495.3**	**496.29**	**513.31**	D	**462.25**	**462.5**	466.75	616	616.33	622	923.49	923.99	932.5	1845.98	1846.97	1863.99	16
3	138.84	139.08	143.34	**184.78**	185.11	190.78	**276.67**	**277.16**	285.67	552.33	**553.31**	570.34	G	373.2	373.45	377.7	**497.26**	**497.59**	503.27	**745.39**	**745.88**	**754.4**	1489.78	1490.76	1507.79	15
4	163.6	163.85	168.11	217.8	218.13	223.81	**326.2**	**326.69**	**335.21**	651.39	**652.38**	**669.4**	V	358.94	359.19	363.45	**478.26**	**478.58**	**484.26**	716.88	717.37	725.89	1432.75	1433.74	1450.76	14
5	192.36	192.61	196.86	256.15	256.47	262.15	**383.71**	**384.21**	**392.72**	766.42	**767.4**	**784.43**	D	334.18	334.42	338.68	**445.23**	**445.56**	**451.24**	**667.35**	**667.84**	**676.35**	1333.69	1334.67	1351.7	13
6	214.12	214.36	218.62	285.16	285.48	291.16	**427.23**	**427.72**	**436.24**	853.45	854.44	871.46	S	305.42	305.67	309.92	**406.89**	**407.22**	**412.89**	**609.83**	**610.33**	**618.84**	1218.66	1219.64	1236.67	12
7	235.88	236.12	240.38	314.17	314.49	320.17	**470.75**	471.24	**479.75**	940.48	941.47	958.5	S	283.66	283.91	288.16	**377.88**	**378.21**	**383.88**	**566.32**	**566.81**	**575.32**	1131.63	1132.61	1149.64	11
8	250.13	250.38	254.63	333.17	333.5	339.18	**499.26**	499.75	508.26	997.51	998.49	1015.52	G	261.9	262.15	266.41	**348.87**	**349.2**	354.87	**522.8**	**523.29**	**531.81**	1044.59	1045.58	1062.61	10
9	289.16	289.4	293.66	**385.21**	**385.54**	**391.21**	**577.31**	**577.8**	**586.31**	1153.61	1154.59	1171.62	R	247.65	247.89	252.15	329.86	330.19	**335.87**	**494.29**	**494.78**	503.3	987.57	988.56	1005.58	9
10	**321.18**	**321.43**	325.68	**427.91**	**428.23**	**433.91**	**641.35**	**641.85**	**650.36**	1281.7	1282.69	1299.71	K	208.62	208.87	**213.13**	**277.83**	278.16	283.83	**416.24**	**416.73**	425.25	831.47	832.46	849.48	8
11	345.44	345.69	**349.95**	**460.26**	**460.58**	466.26	689.88	690.37	698.89	1378.75	1379.74	1396.77	P	176.6	176.85	181.1	235.13	235.46	241.13	352.19	352.68	**361.2**	703.38	704.36	**721.39**	7
12	370.71	370.95	**375.21**	**493.94**	**494.27**	499.94	740.4	740.9	749.41	1479.8	1480.79	1497.81	T	152.34	152.58	156.84	202.78	203.11	208.78	303.67	304.16	**312.67**	606.32	607.31	**624.34**	6
13	**384.96**	**385.21**	389.46	**512.95**	**513.27**	**518.95**	**768.92**	769.41	777.92	1536.82	1537.81	1554.83	G	127.07	127.32	131.58	169.1	169.43	175.1	253.14	253.63	262.15	505.28	506.26	**523.29**	5
14	**416.99**	**417.23**	**421.49**	**555.64**	**555.97**	**561.65**	832.96	833.46	**841.97**	1664.92	1665.9	1682.93	K	112.82	113.07	117.32	150.09	150.42	156.09	224.63	225.12	233.64	448.26	**449.24**	466.27	4
15	431.24	431.49	**435.74**	**574.65**	**574.98**	**580.66**	861.47	861.97	870.48	1721.94	1722.92	1739.95	G	80.8	—	85.3	107.39	—	113.4	160.58	—	169.59	320.16	—	338.17	3
16	**456.01**	**456.25**	**460.51**	**607.67**	**608**	**613.68**	911.01	911.5	920.01	1821.01	1821.99	1839.02	V	66.54	—	71.04	88.38	—	94.39	132.07	—	141.08	263.14	—	281.15	2
	—	—	—	—	—	—	—	—	—	—	—	—	Y	41.77	—	46.28	55.36	—	61.37	82.54	—	91.54	164.07	—	**182.08**	1

chainB :

#	$b^{\prime+4}$	b^{*+4}	b^{+4}	$b^{\prime+3}$	b^{*+3}	b^{+3}	$b^{\prime++}$	b^{*++}	b^{++}	$b^{\prime+}$	b^{*+}	b^{+}	seq	$y^{\prime+4}$	y^{*+4}	y^{+4}	$y^{\prime+3}$	y^{*+3}	y^{+3}	$y^{\prime++}$	y^{*++}	y^{++}	$y^{\prime+}$	y^{*+}	y^{+}	#
1	468.5	468.75	473.01	**624.33**	**624.66**	630.34	936	936.49	945	1870.99	1871.97	1889	K	—	—	—	—	—	—	—	—	—	—	—	—	
	—	—	—	—	—	—	—	—	—	—	—	—	L	29.28	—	33.78	38.7	—	44.71	57.55	—	66.55	114.09	—	132.1	1

Mass of detected product ions are shown in red. Precursor ion charges, score values by MassMatrix (score, pp, pp2, and pptag), m/z of precursor ions, observed molecular weight of the peptides, theoretical molecular weight of the peptide, delta = MW(obs) − MW, and peptide sequence are also shown.
Pair of residues that have the same label ($1 or $2) are predicted to be cross-linked.

Table S8: The lists of detected product ions derived from peptides that were predicted to be cross-linked between PsbP and CP26

Index scan# charge score pp pp$_2$ pp$_{tag}$ m/z MW(obs) MW delta miss Unique sequence + modifications

1459 1088 +3 36 8.4 10.0 7.5 1121.8658 3363.5830 3363.6103 −0.0273 2 √ E($1)SSTPVVDGKQYY FKGAK($1)K($2)F GANCGPE($2)AVW + CaAK(17)

chainA :

#	$b^{\prime+3}$	b^{*+3}	b^{+3}	$b^{\prime++}$	b^{*++}	b^{++}	$b^{\prime+}$	b^{*+}	b^{+}	seq	$y^{\prime+3}$	y^{*+3}	y^{+3}	$y^{\prime++}$	y^{*++}	y^{++}	$y^{\prime+}$	y^{*+}	y^{+}	#
1	668.32	668.65	674.33	**1002**	**1002.5**	**1011**	2003	2003.9	2021	E	1115.9	1116.2	1121.9	1673.3	1673.8	1682.3	3345.6	3346.6	3363.6	M
2	697.34	697.66	703.34	**1045.5**	**1046**	**1054.5**	2090	2091	2108	S	442.55	442.88	448.55	663.32	663.81	672.33	**1325.6**	**1326.6**	**1343.7**	12
3	726.35	726.67	732.35	**1089**	**1089.5**	**1098**	2177	2178	2195	S	413.54	413.87	419.54	619.81	620.3	628.81	**1238.6**	1239.6	**1256.6**	11
4	760.03	760.36	**766.03**	**1139.5**	**1140**	**1148.5**	2278.1	2279.1	2296.1	T	384.53	384.86	390.53	576.29	576.78	585.3	1151.6	1152.6	**1169.6**	10
5	792.38	792.71	798.38	1188.1	1188.6	1197.1	2375.1	2376.1	2393.1	P	350.85	351.17	356.85	525.77	526.26	534.77	**1050.5**	**1051.5**	**1068.5**	9
6	825.4	825.73	**831.41**	**1237.6**	**1238.1**	**1246.6**	2474.2	2475.2	2492.2	V	318.5	318.82	324.5	477.24	477.73	486.25	953.47	954.46	971.48	8
7	858.43	858.75	864.43	**1287.1**	**1287.6**	**1296.1**	2573.3	2574.2	2591.3	V	285.47	285.8	291.48	427.71	428.2	436.71	**854.4**	**855.39**	**872.41**	7
8	896.77	897.1	902.77	**1344.7**	**1345.1**	**1353.7**	2688.3	2689.3	2706.3	D	252.45	252.78	258.45	378.17	378.66	387.18	755.34	756.32	**773.35**	6
9	915.77	916.1	921.78	**1373.2**	**1373.7**	**1382.2**	2745.3	2746.3	2763.3	G	214.11	214.44	220.11	320.66	321.15	329.66	640.31	641.29	**658.32**	5
10	958.47	958.8	964.48	1437.2	1437.7	**1446.2**	2873.4	2874.4	2891.4	K	195.1	195.43	201.1	292.15	292.64	301.15	583.29	584.27	601.3	4
11	**1001.2**	**1001.5**	**1007.2**	**1501.2**	**1501.7**	**1510.2**	3001.5	3002.5	3019.5	Q	152.4	152.73	158.41	228.1	228.59	237.11	**455.19**	456.18	473.2	3
12	**1055.5**	**1055.8**	**1061.5**	1582.8	1583.3	**1591.8**	3164.5	3165.5	3182.5	Y	109.72	—	115.72	164.07	—	173.08	327.13	—	345.14	2
	—	—	—	—	—	—	—	—	—	Y	55.36	—	61.37	82.54	—	91.54	164.07	—	182.08	1

chainB :

#	$b^{\prime+3}$	b^{*+3}	b^{+3}	$b^{\prime++}$	b^{*++}	b^{++}	$b^{\prime+}$	b^{*+}	b^{+}	seq	$y^{\prime+3}$	y^{*+3}	y^{+3}	$y^{\prime++}$	y^{*++}	y^{++}	$y^{\prime+}$	y^{*+}	y^{+}	#
1	—	—	50.03	—	—	74.54	—	—	148.08	F	—	—	—	—	—	—	—	—	—	
2	—	—	107.06	—	—	160.09	—	—	319.18	K	1066.9	1067.2	1072.9	1599.8	1600.3	1608.8	3198.5	3199.5	3216.5	6
3	—	—	126.07	—	—	188.6	—	—	376.2	G	**1009.8**	1010.1	**1015.8**	1514.2	1514.7	1523.2	3027.4	3028.4	3045.4	5
4	—	—	149.75	—	—	224.12	—	—	447.24	A	990.81	991.14	**996.81**	1485.7	1486.2	**1494.7**	2970.4	2971.4	2988.4	4
5	671	671.33	677.01	**1006**	**1006.5**	**1015**	2011	2012	2029	K	967.13	967.46	973.13	1450.2	1450.7	1459.2	2899.4	2900.4	2917.4	3
6	**1060.9**	**1061.2**	1066.9	1590.8	**1591.3**	1599.8	3180.5	3181.5	3198.5	K	439.87	440.2	445.88	659.31	659.8	668.31	1317.6	1318.6	**1335.6**	2
	—	—	—	—	—	—	—	—	—	F	50.03	—	56.03	74.54	—	83.55	148.08	—	166.09	1

chainC :

#	$b^{\prime+3}$	b^{*+3}	b^{+3}	$b^{\prime++}$	b^{*++}	b^{++}	$b^{\prime+}$	b^{*+}	b^{+}	seq	$y^{\prime+3}$	y^{*+3}	y^{+3}	$y^{\prime++}$	y^{*++}	y^{++}	$y^{\prime+}$	y^{*+}	y^{+}	#
1	—	—	20.01	—	—	29.52	—	—	58.03	G	—	—	—	—	—	—	—	—	—	
2	—	—	43.69	—	—	65.04	—	—	129.07	A	1096.9	1097.2	**1102.9**	1644.8	1645.3	1653.8	3288.6	3289.6	3306.6	9
3	—	76.03	81.71	—	113.54	122.06	—	226.08	243.11	N	1073.2	1073.5	**1079.2**	1609.3	1609.8	1618.3	3217.5	3218.5	3235.6	8
4	—	129.38	135.05	—	193.56	202.07	—	386.11	403.14	C	1035.2	1035.5	**1041.2**	1552.3	1552.7	1561.3	3103.5	3104.5	3121.5	7
5	—	148.38	154.06	—	222.07	230.58	—	443.13	460.16	G	981.83	982.16	**987.83**	**1472.2**	**1472.7**	**1481.2**	2943.5	2944.5	2961.5	6
6	—	180.73	186.41	—	270.6	279.11	—	540.19	557.21	P	962.82	963.15	968.82	1443.7	1444.2	1452.7	2886.5	2887.4	2904.5	5
7	991.14	991.47	**997.14**	1486.2	1486.7	1495.2	2971.4	2972.4	2989.4	E	930.47	930.8	936.47	1395.2	1395.7	1404.2	2789.4	2790.4	2807.4	4
8	**1014.8**	**1015.2**	1020.8	1521.7	1522.2	1530.7	3042.4	3043.4	3060.5	A	119.74	—	125.74	179.1	—	188.1	357.19	—	375.2	3
9	**1047.8**	**1048.2**	**1053.8**	1571.3	1571.8	1580.3	3141.5	3142.5	3159.5	V	96.06	—	102.06	143.58	—	152.59	286.16	—	304.17	2
	—	—	—	—	—	—	—	—	—	W	63.03	—	69.04	94.05	—	103.05	187.09	—	205.1	1

Mass of detected product ions are shown in red. Precursor ion charges, score values by MassMatrix (score, pp, pp2, and pptag), m/z of precursor ions, observed molecular weight of the peptides, theoretical molecular weight of the peptide, delta = MW(obs) − MW, and peptide sequence are also shown. Pair of residues that have the same label ($1 or $2) are predicted to be cross-linked.