The interaction interface of Mason-Pfizer monkey virus matrix and envelope proteins.

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Running Title: Direct interaction between M-PMV matrix protein and Env

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J. P. and J. S. contributed equally to this work

Supplementary figures and tables:

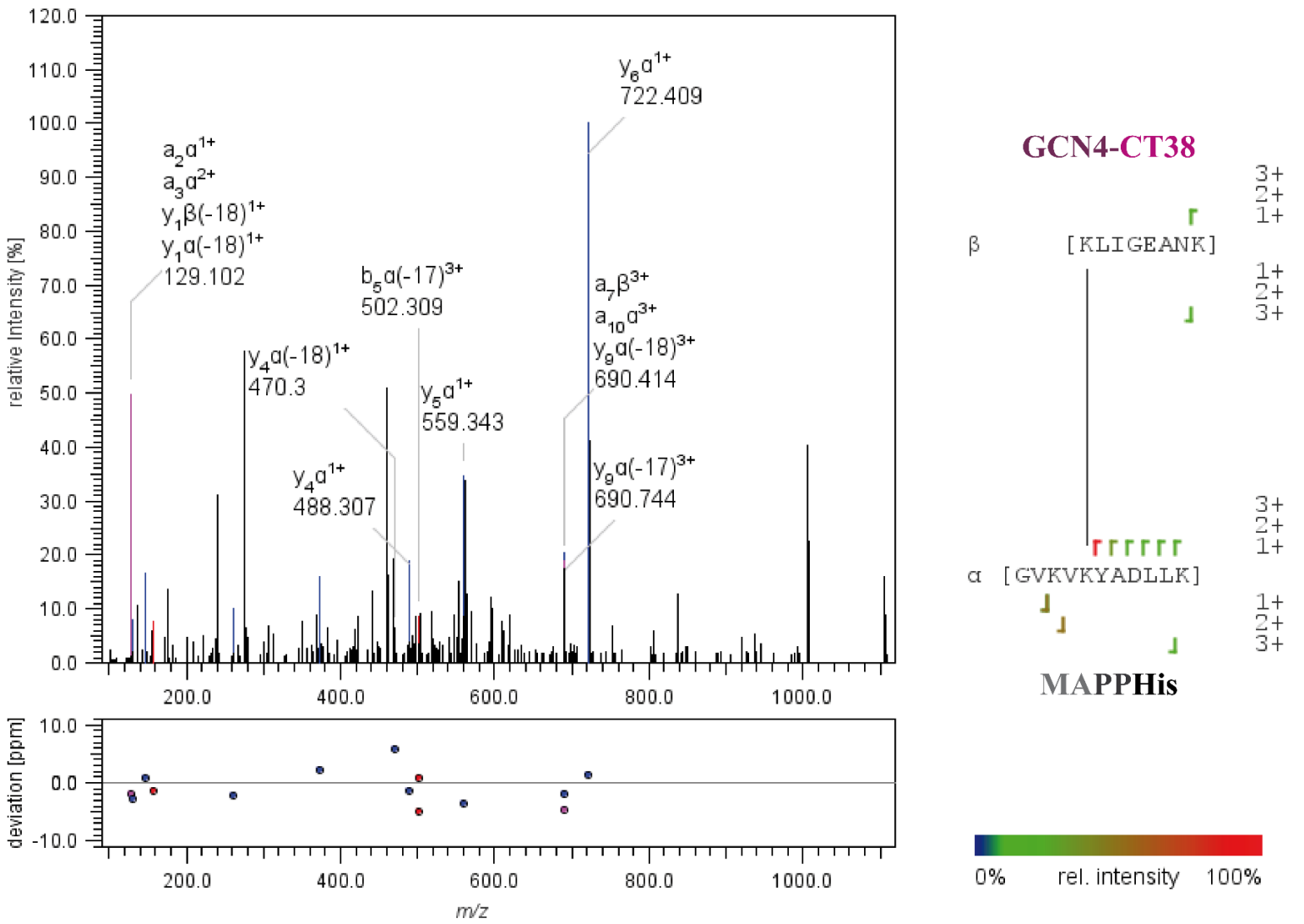

Figure S1: The fragmentation spectrum of the K27-K27 (GCN4-CT38 to MAPPHis) cross-link. The experimental mass of the precursor with the charge $[M+H]^+$ = 2243.336 Da; calculated mass = 2243.337 Da; mass deviation = −0.67 ppm; m/z value = 561.589; charge = +4; calculated sequence coverage: 53%; StavroX score = 51. The cross-link sequence is on the right. The longer peptide is labelled as α peptide and the shorter one as β peptide according to the widely used nomenclature of cross-links. All identified fragment ions are displayed in sequence by symbols for the b- or y- type of ions with their charge state and colored by their relative intensity (the range is displayed below the sequence). In the fragmentation spectra, a-type ions are in orange, b-type ions are in red, y-type ions are in blue and the precursor ion is in light green (if presented). The signals assigned as both a- and y-type ions are in purple. The only matched signals are displayed in the spectra and are characterized by type, mass and charge (the numbers in the parentheses show the neutral losses during the fragmentation if they occur). The mass-deviation plot is presented as spots below the spectrum with the range in ppm.

Table S1: Identified fragment ions of K27-K27 cross-link (Figure S1). The only identified fragments in spectrum of K27-K27 cross-link are presented and characterized by absolute intensity, relative intensity, experimental m/z value, calculated m/z value, mass deviation in ppm, ion type, charge state, peptide type and masses of neutral losses if they occur. The longer peptide of cross-link is labelled as α peptide and the shorter one as β peptide according to the widely used nomenclature of cross-links. The ion type column contains a-, b- or y-type of ions according to the widely used nomenclature in peptide fragmentation pathways or abbreviation P0 for precursor ion (if presented)). The last column shows loss of ammonia (-17 Da), water (-18 Da) or higher values depends on their multiplicities (if neutral loss/losses is/are presented).

absolute intensity	relative intensity	m/z value [Da]	calculated m/z [Da]	mass deviation [ppm]	ion type	charge state	peptide type	neutral loss [Da]
60999	68.4	129.1023	129.1022	0.6604	a2	1	α	0
60999	68.4	129.1023	129.1022	0.6604	a3	2	α	0
60999	68.4	129.1023	129.1022	0.6604	y1	1	β	18
60999	68.4	129.1023	129.1022	0.6604	y1	1	α	18
11849.1	13.3	130.0859	130.0863	-2.4923	y1	1	β	17
11849.1	13.3	130.0859	130.0863	-2.4923	y1	1	α	17
23367.4	26.2	147.1123	147.1128	-3.275	y1	1	β	0
23367.4	26.2	147.1123	147.1128	-3.275	y1	1	α	0
7456.7	8.4	157.0958	157.0971	-8.3384	b2	1	α	0
13677.2	15.3	260.1969	260.1969	0.3054	y2	1	α	0
13209.1	14.8	356.2531	356.2543	-3.6083	y3	1	α	17
20699.7	23.2	373.2786	373.2808	-6.3704	y3	1	α	0
17975.8	20.1	488.3072	488.3079	-1.3209	y4	1	α	0
14499.5	16.3	501.9784	501.9801	-3.4649	b5	3	α	18
12838.3	14.4	502.3101	502.3081	4.0314	b5	3	α	17
12773.8	14.3	557.3364	557.3332	5.7968	P0	4		17
34527.7	38.7	559.3433	559.345	-3.0953	y5	1	α	0
28184.2	31.6	690.4132	690.4171	-5.6795	a7	3	β	0
28184.2	31.6	690.4132	690.4171	-5.6795	a10	3	α	0
28184.2	31.6	690.4132	690.4171	-5.6795	y9	3	α	18
36119.8	40.5	690.7442	690.7452	-1.2799	y9	3	α	17
89226.4	100	722.4092	722.4083	1.2782	y6	1	α	0

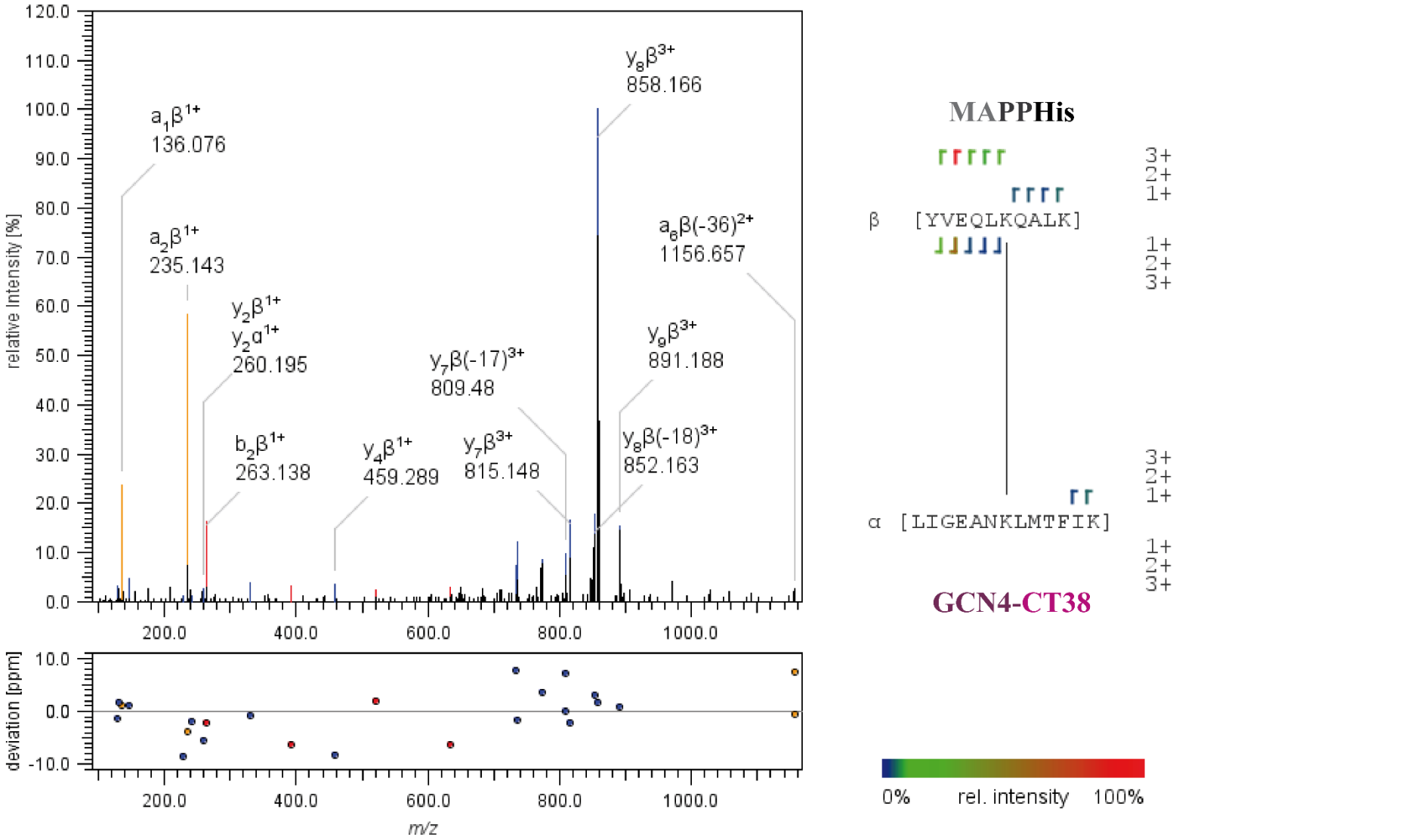

Figure S2: The fragmentation spectrum of the K34-K16 (GCN4-CT38 to MAPPHis) cross-link. The experimental mass of the precursor with the charge $[M+H]^+$ = 2834.615 Da; calculated mass = 2834.610 Da; mass deviation = 1.90 ppm; m/z value = 709.409; charge = +4; calculated sequence coverage: 52%; StavroX score = 87. The cross-link sequence is on the right. The longer peptide is labelled as α peptide and the shorter one as β peptide according to the widely used nomenclature of cross-links. All identified fragment ions are displayed in sequence by symbols for the b- or y- type of ions with their charge state and colored by their relative intensity (the range is displayed below the sequence). In the fragmentation spectra, a-type ions are in orange, b-type ions are in red, y-type ions are in blue and the precursor ion is in light green (if presented). The only matched signals are displayed in the spectra and are characterized by type, mass and charge (the numbers in the parentheses show the neutral losses during the fragmentation if they occur). The mass-deviation plot is presented as spots below the spectrum with the range in ppm.

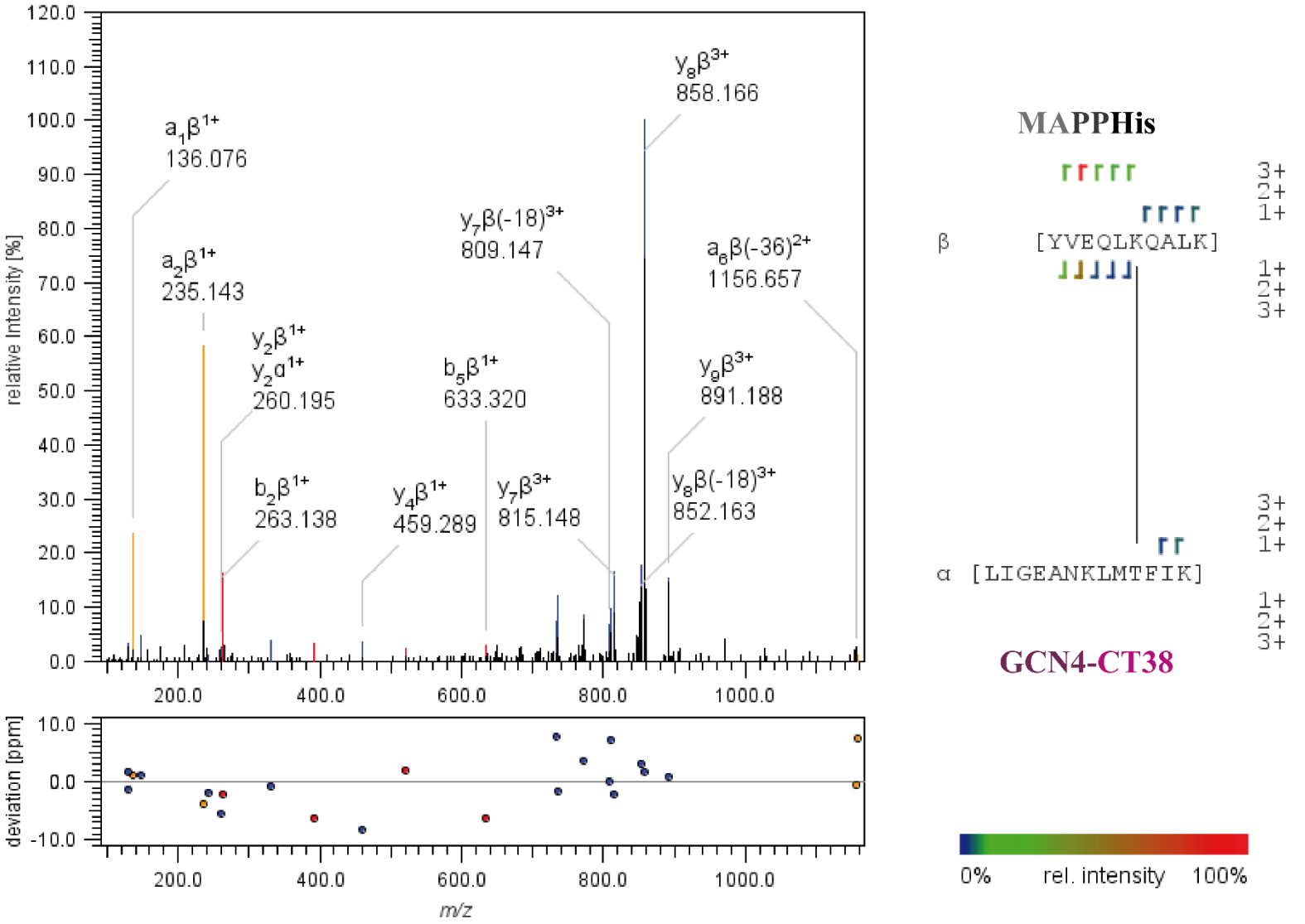

Figure S3: The fragmentation spectrum of the T37-K16 (GCN4-CT38 to MAPPHis) cross-link. The experimental mass of the precursor with the charge $[M+H]^+$ = 2834.615 Da; calculated mass = 2834.610 Da; mass deviation = 1.90 ppm; m/z value = 709.409; charge = +4; calculated sequence coverage: 52%; StavroX score = 86. The cross-link sequence is on the right. The longer peptide is labelled as α peptide and the shorter one as β peptide according to the widely used nomenclature of cross-links. All identified fragment ions are displayed in sequence by symbols for the b- or y- type of ions with their charge state and colored by their relative intensity (the range is displayed below the sequence). In the fragmentation spectra, a-type ions are in orange, b-type ions are in red, y-type ions are in blue and the precursor ion is in light green (if presented). The only matched signals are displayed in the spectra and are characterized by type, mass and charge (the numbers in the parentheses show the neutral losses during the fragmentation if they occur). The mass-deviation plot is presented as spots below the spectrum with the range in ppm.

Table S2: Identified fragment ions of K34-K27 cross-link (Figure S2) or T37-K27 cross-link (Figure S3). The only identified fragments in spectrum of K27-K27 cross-link are presented and characterized by absolute intensity, relative intensity, experimental m/z value, calculated m/z value, mass deviation in ppm, ion type, charge state, peptide type and masses of neutral losses if they occur. The longer peptide of cross-link is labelled as α peptide and the shorter one as β peptide according to the widely used nomenclature of cross-links. The ion type column contains a-, b- or y-type of ions according to the widely used nomenclature in peptide fragmentation pathways or abbreviation P0 for precursor ion (if presented)). The last column shows loss of ammonia (-17 Da), water (-18 Da) or higher values depends on their multiplicities (if neutral loss/losses is/are presented).

absolute intensity	relative intensity	m/z value [Da]	calculated m/z [Da]	mass deviation [ppm]	ion type	charge state	peptide type	neutral loss [Da]
16953.7	3.3	129.1021	129.1022	-1.283	y1	1	β	18
16953.7	3.3	129.1021	129.1022	-1.283	y1	1	α	18
10121.8	1.9	130.0865	130.0863	1.7518	y1	1	β	17
10121.8	1.9	130.0865	130.0863	1.7518	y1	1	α	17
123904.5	23.8	136.0759	136.0757	1.2342	a1	1	β	0
24683.7	4.7	147.113	147.1128	1.025	y1	1	β	0
24683.7	4.7	147.113	147.1128	1.025	y1	1	α	0
6558.4	1.3	229.1183	229.1203	-8.5002	y4	2	α	51
304062.9	58.5	235.1432	235.1441	-3.7161	a2	1	β	0
6871.2	1.3	242.1859	242.1863	-1.8249	y2	1	β	18
6871.2	1.3	242.1859	242.1863	-1.8249	y2	1	α	18
14540.9	2.8	260.1954	260.1969	-5.4633	y2	1	β	0
14540.9	2.8	260.1954	260.1969	-5.4633	y2	1	α	0
84348	16.2	263.1385	263.139	-2.1476	b2	1	β	0
19805.5	3.8	331.2337	331.234	-0.7118	y3	1	β	0
17236.4	3.3	392.1791	392.1816	-6.2913	b3	1	β	0
19100.5	3.7	459.2888	459.2926	-8.2111	y4	1	β	0
12614.2	2.4	520.2411	520.2402	1.8085	b4	1	β	0
14802	2.8	633.3202	633.3243	-6.3677	b5	1	β	0
38626.5	7.4	734.436	734.4304	7.6613	y7	3	α	36
62711.1	12.1	734.768	734.7692	-1.6173	y5	3	β	0
44500	8.6	772.4666	772.4639	3.5526	y6	3	β	0
36088.4	6.9	809.1464	809.1466	-0.0233	y7	3	β	18
50288.8	9.7	809.4803	809.4746	7.0578	y7	3	β	17
85494.1	16.4	815.1484	815.15	-2.0717	y7	3	β	0
92956.4	17.9	852.1632	852.1607	2.9267	y8	3	β	18
519846.6	100	858.1657	858.1643	1.6844	y8	3	β	0
80249.6	15.4	891.1878	891.1871	0.8239	y9	3	β	0
7709.4	1.5	1156.6574	1156.6579	-0.5192	a6	2	β	36
6535.6	1.3	1157.6507	1157.642	7.5403	a6	2	β	34

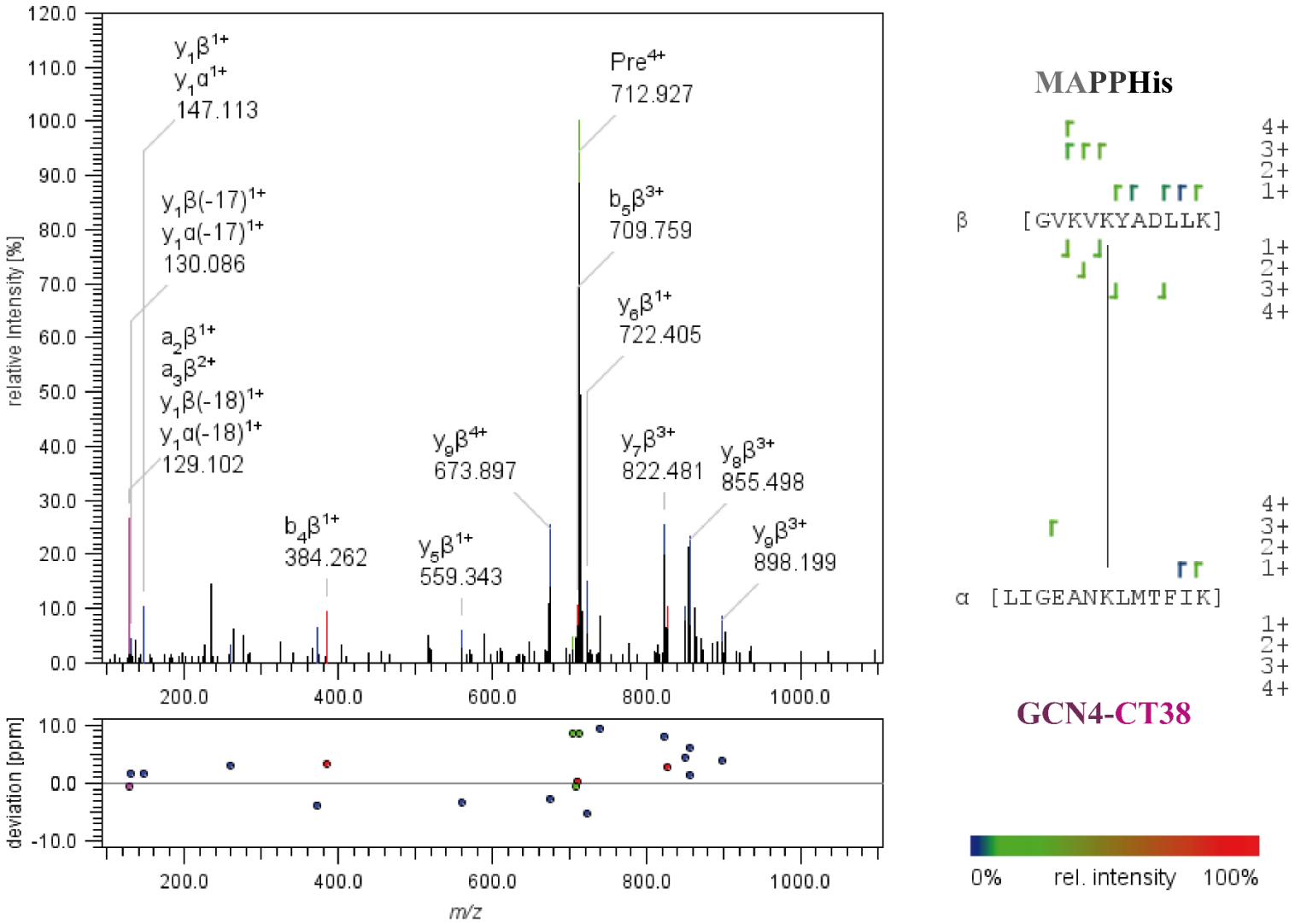

Figure S4: The fragmentation spectrum of the K34-K27 (GCN4-CT38 to MAPPHis) cross-link. The experimental mass of the precursor with the charge $[M+H]^+$ = 2848.674 Da; calculated mass = 2848.662 Da; mass deviation = 4.36 ppm; m/z value = 712.924; charge = +4; calculated sequence coverage: 54%; StavroX score = 57. The cross-link sequence is on the right. The longer peptide is labelled as α peptide and the shorter one as β peptide according to the widely used nomenclature of cross-links. All identified fragment ions are displayed in sequence by symbols for the b- or y- type of ions with their charge state and colored by their relative intensity (the range is displayed below the sequence). In the fragmentation spectra, a-type ions are in orange, b-type ions are in red, y-type ions are in blue and the precursor ion is in light green (if presented). The signals assigned as both a- and y-type ions are in purple. The only matched signals are displayed in the spectra and are characterized by type, mass and charge (the numbers in the parentheses show the neutral losses during the fragmentation if they occur). The mass-deviation plot is presented as spots below the spectrum with the range in ppm.

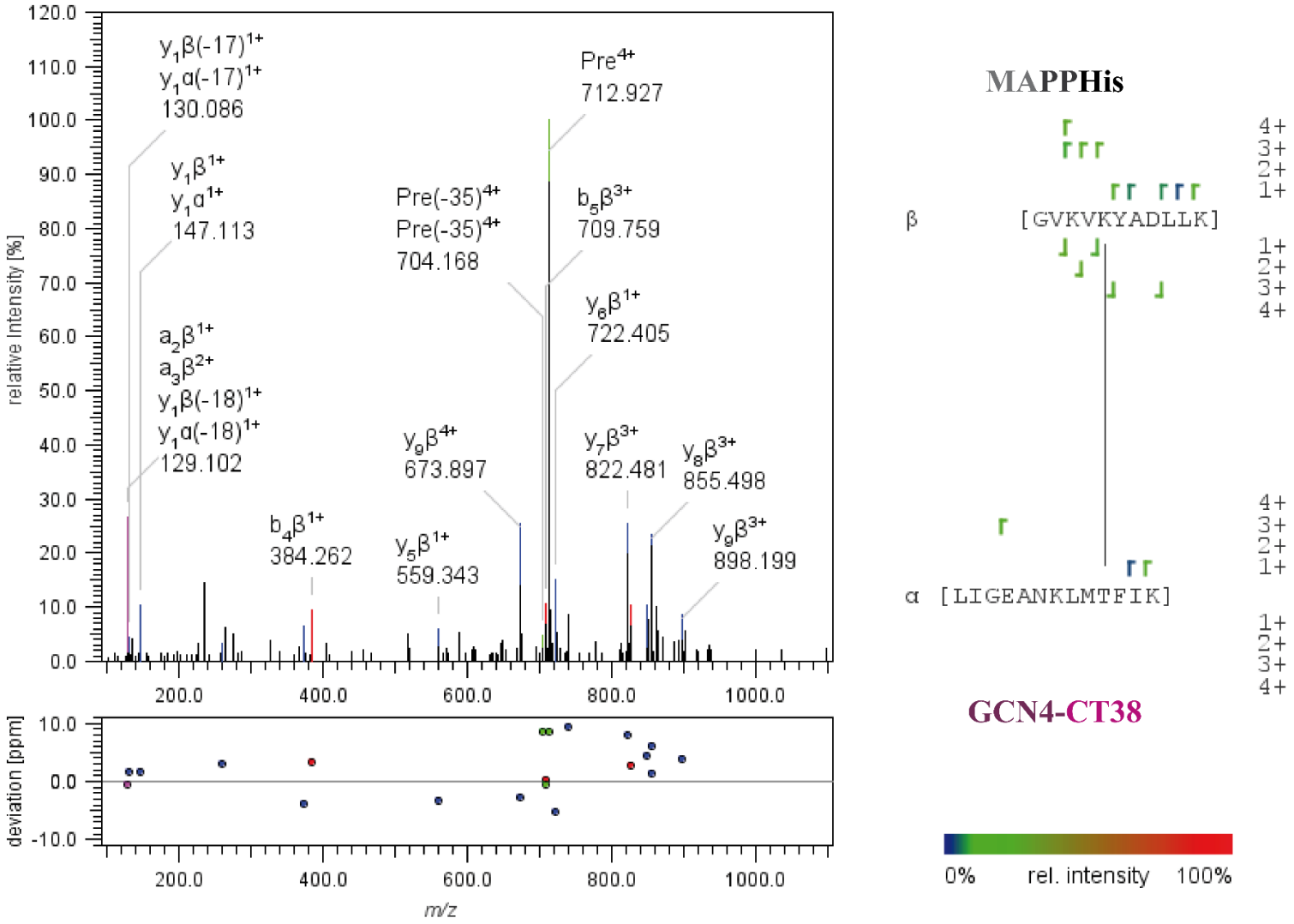

Figure S5: The fragmentation spectrum of the T37-K27 (GCN4-CT38 to MAPPHis) cross-link. The experimental mass of the precursor with the charge $[M+H]^+$ = 2848.674 Da; calculated mass = 2848.662 Da; mass deviation = 4.36 ppm; m/z value = 712.924; charge = +4; calculated sequence coverage: 54%; StavroX score = 116. The sequence of cross-link is on the right. The longer peptide is labelled as α peptide and the shorter one as β peptide according to a widely used nomenclature of cross-links. All identified fragment ions are displayed in sequence by symbols for b- or y- type of ions with their charge state and colored by their relative intensity (the range is displayed under the sequence). In fragmentation spectra a-type ions are in orange, b-type ions are in red, y-type ions are in blue and precursor ion is in light green (if presented). The signals assigned as a-type and y-type ions concurrently are in purple. The only matched signals are displayed in the spectra and are characterized by type, mass and charge (numbers in brackets show the neutral losses during fragmentation if they occur). The mass deviation plot presented as spots is situated under the spectrum with the range in ppm.

Table S3: Identified fragment ions of K34-K27 cross-link (Figure S4) or T37-K27 cross-link (Figure S5). The only identified fragments in spectrum of K27-K27 cross-link are presented and characterized by absolute intensity, relative intensity, experimental m/z value, calculated m/z value, mass deviation in ppm, ion type, charge state, peptide type and masses of neutral losses if they occur. The longer peptide of cross-link is labelled as α peptide and the shorter one as β peptide according to the widely used nomenclature of cross-links. The ion type column contains a-, b- or y-type of ions according to the widely used nomenclature in peptide fragmentation pathways or abbreviation P0 for precursor ion (if presented)). The last column shows loss of ammonia (-17 Da), water (-18 Da) or higher values depends on their multiplicities (if neutral loss/losses is/are presented).

absolute intensity	relative intensity	m/z value [Da]	calculated m/z [Da]	mass deviation [ppm]	ion type	charge state	peptide type	neutral loss [Da]
57587.5	26.8	129.1022	129.1022	-0.5394	a2	1	β	0
57587.5	26.8	129.1022	129.1022	-0.5394	a3	2	β	0
57587.5	26.8	129.1022	129.1022	-0.5394	y1	1	β	18
57587.5	26.8	129.1022	129.1022	-0.5394	y1	1	α	18
9248	4.3	130.0865	130.0863	1.7572	y1	1	β	17
9248	4.3	130.0865	130.0863	1.7572	y1	1	α	17
22217.3	10.3	147.113	147.1128	1.6192	y1	1	β	0
22217.3	10.3	147.113	147.1128	1.6192	y1	1	α	0
6803.6	3.2	260.1977	260.1969	3.0541	y2	1	β	0
6803.6	3.2	260.1977	260.1969	3.0541	y2	1	α	0
13786.2	6.4	373.2795	373.2808	-3.7836	y3	1	β	0
20326.9	9.4	384.2618	384.2605	3.2096	b4	1	β	0
12440.6	5.8	559.3432	559.345	-3.2208	y5	1	β	0
54783.8	25.5	673.8967	673.8985	-2.7099	y9	4	β	0
10411.8	4.8	704.1677	704.1617	8.5832	P0	4		35
10411.8	4.8	704.1677	704.1617	8.5832	P0	4		35
10138	4.7	708.6639	708.6643	-0.6727	P0	4		17
23203.3	10.8	709.7587	709.7585	0.4122	b5	3	β	0
215128.2	100	712.927	712.921	8.4164	P0	4		0
32471.8	15.1	722.4045	722.4083	-5.2737	y6	1	β	0
12158.4	5.7	739.1213	739.1144	9.3328	y7	3	α	36
55128.5	25.6	822.4811	822.4743	8.0884	y7	3	β	0
22300.8	10.4	826.1366	826.1343	2.7503	b8	3	β	0
22236.9	10.3	849.4975	849.4937	4.4211	y8	3	β	18
50349.1	23.4	855.4983	855.4972	1.2546	y8	3	β	0
43575.1	20.3	855.8343	855.829	6.1611	y10	3	α	0
18656.7	8.7	898.1991	898.1956	3.9281	y9	3	β	0

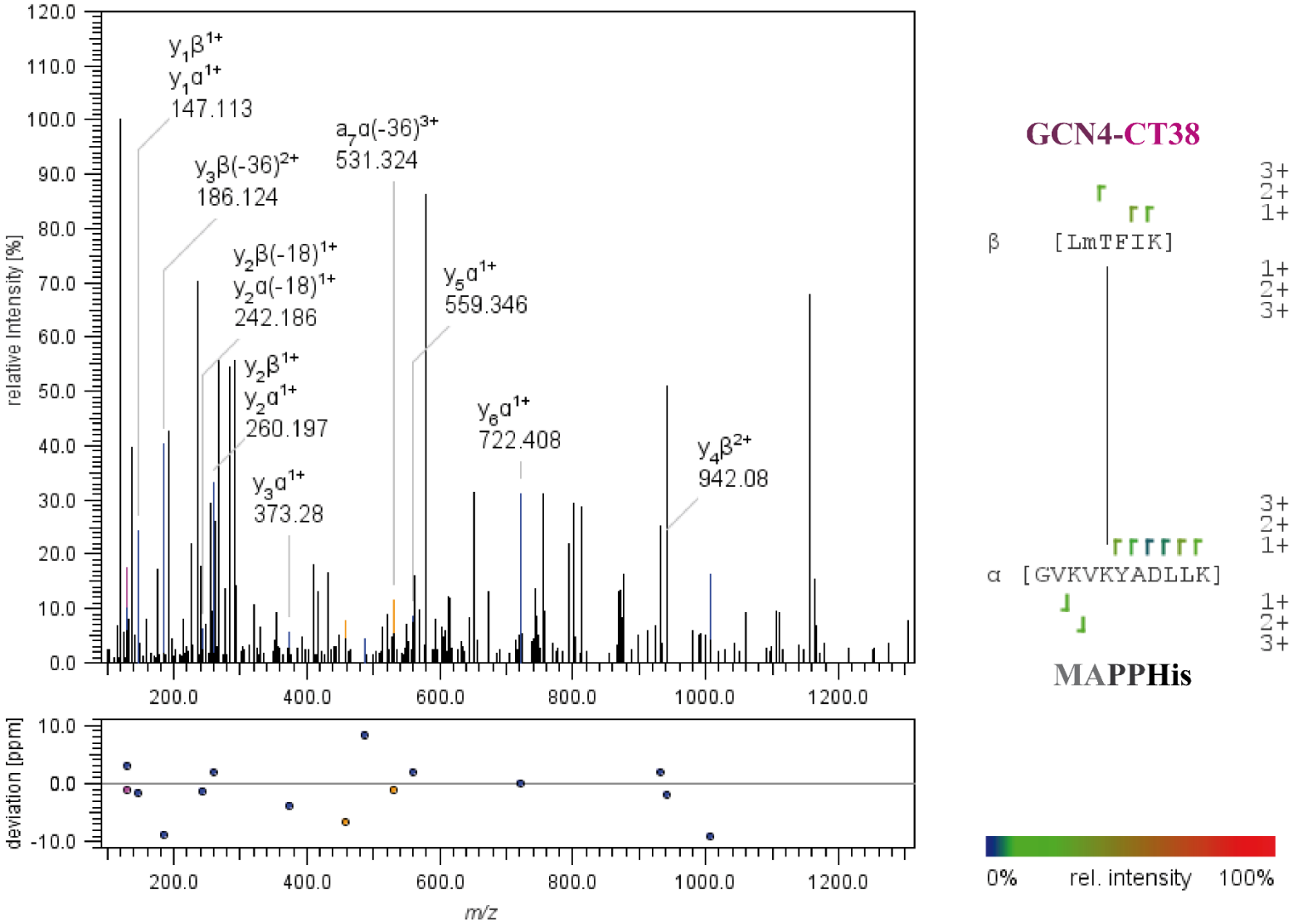

Figure S6: Fragmentation spectrum of T37-K27 (GCN4-CT38 to MAPPHis) cross-link. Experimental mass of precursor with charge $[M+H]^+$ = 2143.276 Da; calculated mass = 2143.275 Da; mass deviation = 0.63 ppm; m/z value = 715.097; charge = +3; calculated sequence coverage: 65%; StavroX score = 80. The sequence of cross-link is on the right. The longer peptide is labelled as α peptide and the shorter one as β peptide according to a widely used nomenclature of cross-links. All identified fragment ions are displayed in sequence by symbols for b- or y- type of ions with their charge state and colored by their relative intensity (the range is displayed under the sequence). In fragmentation spectra a-type ions are in orange, b-type ions are in red, y-type ions are in blue and precursor ion is in light green (if presented). The signals assigned as a-type and y-type ions concurrently are in purple. The only matched signals are displayed in the spectra and are characterized by type, mass and charge (numbers in brackets show the neutral losses during fragmentation if they occur). The mass deviation plot presented as spots is situated under the spectrum with the range in ppm.

Table S4: Identified fragment ions of T37-K27 cross-link (Figure S6). The only identified fragments in spectrum of K27-K27 cross-link are presented and characterized by absolute intensity, relative intensity, experimental m/z value, calculated m/z value, mass deviation in ppm, ion type, charge state, peptide type and masses of neutral losses if they occur. The longer peptide of cross-link is labelled as α peptide and the shorter one as β peptide according to the widely used nomenclature of cross-links. The ion type column contains a-, b- or y-type of ions according to the widely used nomenclature in peptide fragmentation pathways or abbreviation P0 for precursor ion (if presented)). The last column shows loss of ammonia (-17 Da), water (-18 Da) or higher values depends on their multiplicities (if neutral loss/losses is/are presented).

absolute intensity	relative intensity	m/z value [Da]	calculated m/z [Da]	mass deviation [ppm]	ion type	charge state	peptide type	neutral loss [Da]
90228	17.4	129.1021	129.1022	-1.2186	a2	1	α	0
90228	17.4	129.1021	129.1022	-1.2186	a3	2	α	0
90228	17.4	129.1021	129.1022	-1.2186	y1	1	β	18
90228	17.4	129.1021	129.1022	-1.2186	y1	1	α	18
52920.3	10.2	130.0867	130.0863	3.1225	y1	1	β	17
52920.3	10.2	130.0867	130.0863	3.1225	y1	1	α	17
125270	24.2	147.1125	147.1128	-1.5736	y1	1	β	0
125270	24.2	147.1125	147.1128	-1.5736	y1	1	α	0
208502	40.3	186.1241	186.1257	-8.8909	y3	2	β	36
31472.7	6.1	242.186	242.1863	-1.3583	y2	1	β	18
31472.7	6.1	242.186	242.1863	-1.3583	y2	1	α	18
172387	33.3	260.1973	260.1969	1.8404	y2	1	β	0
172387	33.3	260.1973	260.1969	1.8404	y2	1	α	0
29658.8	5.7	373.2795	373.2808	-3.7333	y3	1	α	0
39537.7	7.6	459.2913	459.2943	-6.5686	a5	3	α	18
23124.3	4.5	488.3118	488.3079	8.1373	y4	1	α	0
59919.7	11.6	531.3237	531.3243	-1.0189	a7	3	α	36
43944.7	8.5	559.346	559.345	1.8163	y5	1	α	0
161494	31.2	722.4084	722.4083	0.091	y6	1	α	0
56138.7	10.8	933.0779	933.0761	1.9891	y4	2	β	18
123810	23.9	942.0796	942.0813	-1.8935	y4	2	β	0
84103.7	16.2	1006.5847	1006.5938	-9.0193	y5	2	β	18

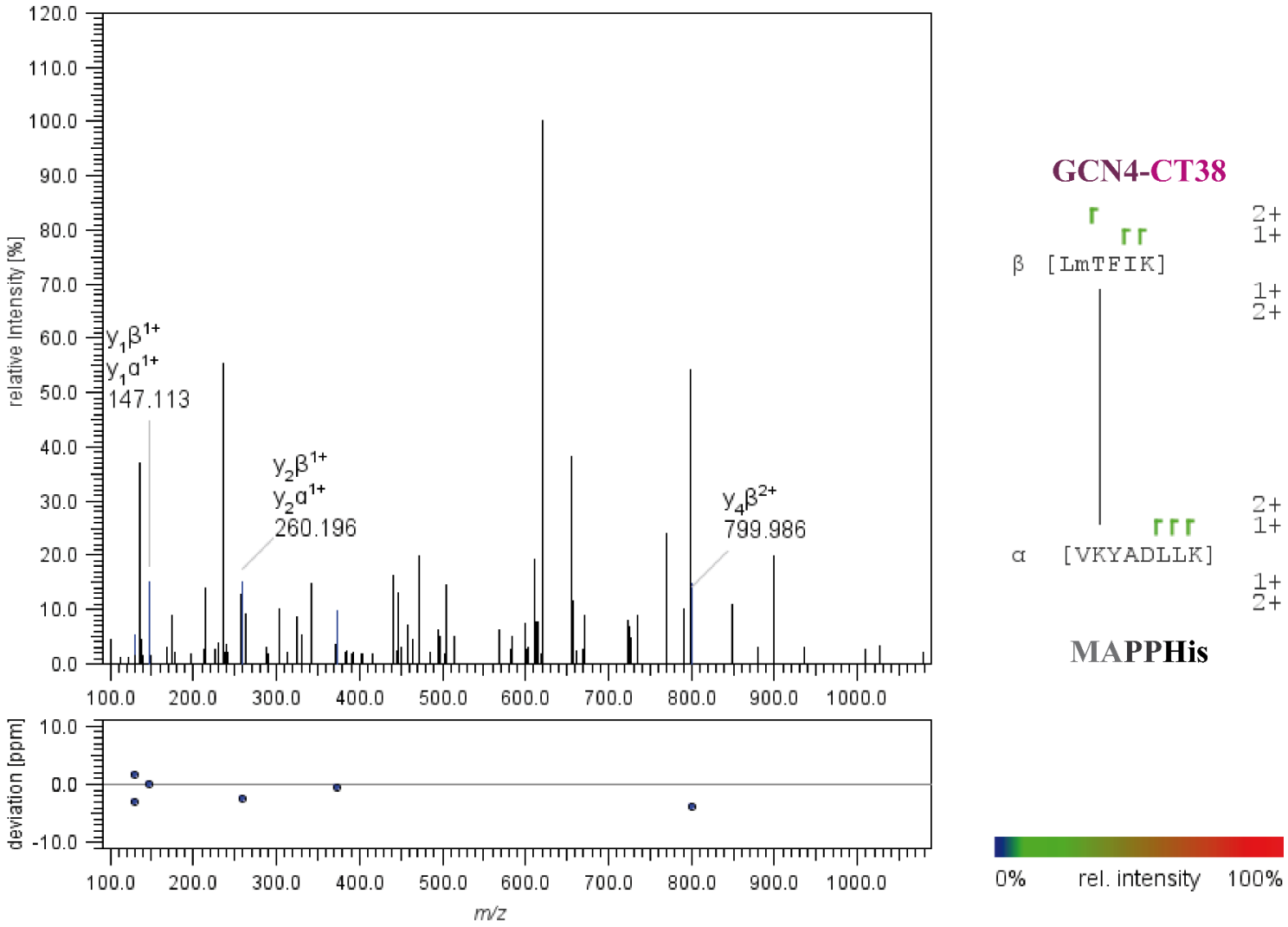

Figure S7: The fragmentation spectrum of the T37-K27 (GCN4-CT38 to MAPPHis) cross-link. The experimental mass of the precursor with the charge $[M+H]^+$ = 1859.087 Da; calculated mass = 1859.090 Da; mass deviation = −1.43 ppm; m/z value = 620.367; charge = +3; calculated sequence coverage: 43%; StavroX score = 43. The cross-link sequence is on the right. The longer peptide is labelled as α peptide and the shorter one as β peptide according to the widely used nomenclature of cross-links. All identified fragment ions are displayed in sequence by symbols for the b- or y- type of ions with their charge state and colored by their relative intensity (the range is displayed below the sequence). In the fragmentation spectra, a-type ions are in orange, b-type ions are in red, y-type ions are in blue and the precursor ion is in light green (if presented). The only matched signals are displayed in the spectra and are characterized by type, mass and charge (the numbers in the parentheses show the neutral losses during the fragmentation if they occur). The mass-deviation plot is presented as spots below the spectrum with the range in ppm.

Table S5: Identified fragment ions of T37 cross-link (Figure S7). The only identified fragments in spectrum of K27-K27 cross-link are presented and characterized by absolute intensity, relative intensity, experimental m/z value, calculated m/z value, mass deviation in ppm, ion type, charge state, peptide type and masses of neutral losses if they occur. The longer peptide of cross-link is labelled as α peptide and the shorter one as β peptide according to the widely used nomenclature of cross-links. The ion type column contains a-, b- or y-type of ions according to the widely used nomenclature in peptide fragmentation pathways or abbreviation P0 for precursor ion (if presented)). The last column shows loss of ammonia (-17 Da), water (-18 Da) or higher values depends on their multiplicities (if neutral loss/losses is/are presented).

absolute intensity	relative intensity	m/z value [Da]	calculated m/z [Da]	mass deviation [ppm]	ion type	charge state	peptide type	neutral loss [Da]
8184.7	5.5	129.1019	129.1022	-3.0127	y1	1	β	18
8184.7	5.5	129.1019	129.1022	-3.0127	y1	1	α	18
7870.5	5.3	130.0865	130.0863	1.5381	y1	1	β	17
7870.5	5.3	130.0865	130.0863	1.5381	y1	1	α	17
22536	15.1	147.1128	147.1128	-0.0162	y1	1	β	0
22536	15.1	147.1128	147.1128	-0.0162	y1	1	α	0
22697.3	15.2	260.1961	260.1969	-2.554	y2	1	β	0
22697.3	15.2	260.1961	260.1969	-2.554	y2	1	α	0
14418.1	9.6	373.2807	373.2808	-0.5247	y3	1	α	0
22060.9	14.7	799.9859	799.9888	-3.8038	y4	2	β	0