Supplementary Information (SI) for Analyst.

Supplementary Tables

Characterization by LC-MS/MS analysis of KLH vaccine conjugated with a tick antigen peptides.

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Table S1. Diagnostic ions originated by the fragmentation of the peptide bond located at the *N*-terminal side of Pro^{11} [1] in Cys^{1}pP0 peptides that were used to validate the assignment of the type 2 peptides performed by Kojak [2] and pLink2 [3] software. These fragment ions provide information on the number of amino acids of the proteolytic fragment of Cys^{1}pP0 in the structures of all assigned type 2 peptides

#	**Cys^{1}pP0**	**$y"_{n\ (\alpha\ or\ \beta)}$**	**m ($y"_n$)**
1	(1-14)	$y"_3$	374.1563
2	(1-16)	$y"_5$	589.2833
3	(1-17)	$y"_6$	717.3782

Table S2. Diagnostic ions named as C+L correspond to the fragmentation of the pseudopeptide bond between the linker and the epsilon amino group of Lys residues present in all type 2 peptides with transcyclized linker that contain in their structures different proteolytic fragments of Cys^{1}pP0 peptide (see **Fig. S2** and **Fig. S3**). C means the different proteolytic fragments of the Cys^{1}pP0 peptide linked by a pseudopeptide bond to the transcyclized linker named L ($+C_7H_6NO_3$) in this manuscript. C+L fragment ion is considered a b_n ion type, and the 2+ is due to the addition of one proton and the carbonyl group with a positive charge ($-C{\equiv}O^{\oplus}$).

#	**Cys^{1}pP0**	**C+L**	
		Global formula	**m/z**
1	(1-11)	$C_{40}H_{63}N_{13}O_{15}S_1$	499.7222 (2+) / 998.4366 (1+)
2	(1-14)	$C_{55}H_{84}N_{16}O_{22}S_1$	677.2911 (2+) / 1353.5744 (1+)
3	(1-16)	$C_{64}H_{102}N_{19}O_{25}S_1$	784.8547 (2+) / 1568.7016 (1+)
4	(1-17)	$C_{70}H_{113}N_{21}O_{26}S_1$	848.9022 (2+) / 1696.7966 (1+)

Table S3. The diagnostic ion named as C+80 corresponds to the fragmentation of the new pseudopeptide bond originated after the transcyclization process that transforms the thiosuccinimide linker into transcyclized (**Fig. S2** and **Fig. S3**). C corresponds to different proteolytic fragments of the Cys^{1}pP0 peptide. The C+80 fragment ion is exclusive of transcyclized linker, and also provides information on the number of amino acids present in the proteolytic fragment of Cys^{1}pP0 for all type 2 peptides assigned with transcyclized linker.

#	Cys[1]pP0	C+80	
		Global formula	**m/z**
1	(1-11)	$C_{37}H_{58}N_{12}O_{14}S_1$	464.2036 (2+) / 927.3994 (1+)
2	(1-14)	$C_{52}H_{79}N_{15}O_{21}S_1$	641.7726 (2+) / 1282.5374 (1+)
3	(1-16)	$C_{61}H_{96}N_{18}O_{24}S_1$	749.3361 (2+) / 1497.6644 (1+)
4	(1-17)	$C_{67}H_{108}N_{20}O_{25}S_1$	813.3836 (2+) / 1625.7594 (1+)

Table S4. Diagnostic ions named as C+L_h corresponding to the fragmentation of the pseudopeptide bond between the linker and the epsilon amino group of Lys residues present in all type 2 peptides that contain in their structures different proteolytic fragments of Cys[1]pP0 peptide and two structural variants of the linker: hydrolyzed thiosuccinimide linkers (see **Fig. S2** and **Fig. S4**). C means the different proteolytic fragments of the Cys[1]pP0 peptide linked by a pseudopeptide bond to the hydrolyzed thiosuccinimide linkers named as L (+$C_7H_7NO_4$) in this manuscript. C+L_h fragment ion is considered a b_n ion type, and the 2+ is due to the addition of one proton and the carbonyl group with a positive charge (-C≡$O^{\oplus}$).

#	Cys[1]pP0	C+L_h	
		Global formula	**m/z**
1	(1-11)	$C_{40}H_{65}N_{13}O_{16}S_1$	508.7275 (2+) / 1016.4471 (1+)
2	(1-14)	$C_{55}H_{86}N_{16}O_{23}S_1$	686.2964 (2+) / 1371.5851 (1+)
3	(1-16)	$C_{64}H_{104}N_{19}O_{26}S_1$	794.3638 (2+) / 1587.7198 (1+)
4	(1-17)	$C_{70}H_{115}N_{21}O_{27}S_1$	857.9074 (2+) / 1714.8070 (1+)

Table S5. The diagnostic ion named as C+98 corresponds to the fragmentation of the new pseudopeptide bond originated after the hydrolysis process that transforms the thiosuccinimide linker into hydrolyzed thiosuccinimide linkers (**Fig. S2** and **Fig. S4**). C corresponds to different proteolytic fragments of the Cys[1]pP0 peptide. The C+98 fragment ion is exclusive of hydrolyzed thiosuccinimide linkers, and also provides information on the number of amino acids present in the proteolytic fragment of Cys[1]pP0 for all type 2 peptides assigned with hydrolyzed thiosuccinimide linkers.

#	Cys[1]pP0	C+98	
		Global formula	**m/z**
1	(1-11)	$C_{37}H_{60}N_{12}O_{15}S_1$	473.2089 (2+) / 945.4100 (1+)
2	(1-14)	$C_{52}H_{81}N_{15}O_{22}S_1$	650.7779 (2+) / 1300.5480 (1+)
3	(1-16)	$C_{61}H_{98}N_{18}O_{25}S_1$	758.3414 (2+) / 1515.6749 (1+)
4	(1-17)	$C_{67}H_{110}N_{20}O_{26}S_1$	822.3889 (2+) / 1643.7699 (1+)

Table S6. Identification of conjugation sites in KLH1-Cys[1]pP0 conjugate using Kojak [2] and pLink2 [3] software. Type 2 peptides were identified using transcyclized and hydrolyzer linker.

#	*m/z* exp.	*m/z* theor.	*z*	Elemental composition	Assignment [1)]	pLink [2)]	Kojak [3)]	Conjugation site [4)]
1	878.4431	878.4445	2	$C_{72}H_{122}N_{24}O_{25}S_1$	[1-6] [5)]		X	Nt
2	585.9651	585.9656	3				X	
3	582.2919	582.2917	4	$C_{96}H_{160}N_{30}O_{35}S_1$	[1-6]		X	
4	466.0280	466.0355	5				X	
5	795.3931	795.4009	4	$C_{133}H_{220}N_{40}O_{48}S_1$	[6-24] [5)]		X	K6
6	937.9585	937.9672	4	$C_{157}H_{258}N_{46}O_{58}S_1$	[6-24]		X	
7	750.5697	750.5753	5				X	
8	615.2849	615.2916	5	$C_{127}H_{202}N_{40}O_{45}S_2$	[38-52] [6)]	X	X	K51
9	571.7819	571.7897	4	$C_{94}H_{158}N_{30}O_{34}S_1$	[79-84]		X	K83
10	571.9575	571.9615	3	$C_{70}H_{120}N_{24}O_{24}S_1$	[79-84] [5)]	X		
11	742.5496	742.5563	5	$C_{163}H_{242}N_{46}O_{52}S_1$	[118-134]	X	X	K133
12	618.9582	618.9650	6				X	
13	746.1531	746.1584	5	$C_{163}H_{244}N_{46}O_{53}S_1$	[118-134] [7)]		H	
14	785.3786	785.3773	4	$C_{139}H_{204}N_{40}O_{42}S_1$	[118-134] [5)]		X	
15	628.4973	628.5034	5			X	X	
16	655.0707	655.0695	4	$C_{111}H_{177}N_{31}O_{40}S_1$	[126-134]	X	X	
17	682.9968	683.0025	3	$C_{87}H_{139}N_{25}O_{30}S_1$	[126-134] [5)]	X	X	
18	527.4250	527.4308	6	$C_{132}H_{215}N_{41}O_{47}S_1$	[134-146]	X	X	K134
19	632.7104	632.7156	5			X	X	
20	790.6339	790.6432	4			X	X	
21	648.0708	648.0770	4	$C_{108}H_{177}N_{35}O_{37}S_1$	[134-146] [5)]	X	X	
22	522.2539	522.2550	4	$C_{84}H_{140}N_{28}O_{32}S_1$	[134-137]		X	
23	587.6332	587.6382	3	$C_{77}H_{125}N_{21}O_{24}S_1$	[143-148] [5)]	X	X	K146
24	583.5411	583.5467	4	$C_{101}H_{163}N_{27}O_{34}S_1$	[143-148]	X		
25	777.7212	777.7271	3			X		
26	588.0424	588.0499	4	$C_{101}H_{165}N_{27}O_{35}S_1$	[143-148] [7)]		H	
27	652.5242	652.5298	5	$C_{137}H_{224}N_{42}O_{48}S_1$	[135-148]	X	X	
28	543.9350	543.9428	6				X	
29	672.8362	672.8441	4	$C_{113}H_{186}N_{36}O_{38}S_1$	[135-148] [5)]		X	
30	538.4708	538.4768	5			X	X	
31	1095.5075	1095.5154	4	$C_{185}H_{292}N_{52}O_{65}S_3$	[147-170] [6)]	X	X	K148
32	876.6099	876.6139	5				X	
33	1099.5063	1099.5142	4	$C_{185}H_{292}N_{52}O_{66}S_3$	[147-170] [6,8)]		X	
34	879.8086	879.8123	5			X	X	
35	880.2071	880.2160	5	$C_{185}H_{294}N_{52}O_{66}S_3$	[147-170] [6,7)]		H	
36	952.9450	952.9492	4	$C_{161}H_{254}N_{46}O_{55}S_3$	[147-170] [6,5)]	X	X	

37	762.5601	762.5609	5				X	
38	957.4440	957.4518	4	$C_{161}H_{256}N_{46}O_{56}S_3$	[147-170] [5,6,7)]		H	
39	766.1576	766.1630	5				H	
40	765.7520	765.7599	5	$C_{161}H_{254}N_{46}O_{56}S_3$	[147-170] [6,5,8)]		X	
41	956.9401	956.9479	4				X	
42	711.8349	711.8405	4	$C_{119}H_{190}N_{36}O_{41}S_2$	[147-157]	X	X	
43	569.6671	569.6744	5				X	
44	572.8731	572.8734	5	$C_{119}H_{190}N_{36}O_{42}S_2$	[147-157] [8)]		X	
45	569.2675	569.2748	4	$C_{95}H_{152}N_{30}O_{31}S_2$	[147-157] [5)]	X		
46	573.2675	573.2730	4	$C_{95}H_{152}N_{30}O_{32}S_2$	[147-157] [5,8)]	X	X	
47	766.6697	766.6766	3	$C_{98}H_{148}N_{26}O_{34}S_2$	[168-172] [6)]		X	K170
48	804.9795	804.9852	5	$C_{173}H_{266}N_{50}O_{57}S_2$	[177-198]	X	X	
49	863.4078	863.4134	4	$C_{149}H_{228}N_{44}O_{47}S_2$	[177-198] [5)]	X		K189
50	690.9272	690.9327	5			X		
51	694.1261	694.1317	5	$C_{149}H_{228}N_{44}O_{48}S_2$	[177-198] [5,8)]	X		
52	723.6800	723.6796	3	$C_{89}H_{145}N_{27}O_{34}S_1$	[228-232]		X	K229
53	543.0110	543.0115	4				X	
54	838.6378	838.6405	4	$C_{138}H_{223}N_{41}O_{50}S_3$	[230-244] [6)]	X		
55	842.6319	842.6398	4	$C_{138}H_{223}N_{41}O_{51}S_3$	[230-244] [6,8)]		X	
56	674.3055	674.3134	5				X	
57	843.1373	843.1437	4	$C_{138}H_{225}N_{41}O_{51}S_3$	[230-244] [6,7)]		H	K232
58	674.7166	674.7166	5				H	
59	927.7682	927.7639	3	$C_{114}H_{185}N_{35}O_{40}S_3$	[230-244] [6,5)]		X	
60	700.0668	700.0735	4	$C_{114}H_{185}N_{35}O_{41}S_3$	[230-244] [6,5,8)]		X	
61	788.1407	788.1486	5	$C_{164}H_{250}N_{46}O_{61}S_3$	[331-351] [6,8)]		X	
62	788.3730	788.3772	4	$C_{136}H_{212}N_{36}O_{46}S_2$	[337-351]	X		
63	860.7427	860.7455	3	$C_{112}H_{174}N_{30}O_{36}S_2$	[337-351] [5)]	X		K337
64	866.0728	866.0772	3	$C_{112}H_{174}N_{30}O_{37}S_2$	[337-351] [5,8)]	X		
65	964.4519	964.4559	3	$C_{125}H_{191}N_{33}O_{44}S_1$	[337-349]	X		
66	1047.702	1047.6991	5	$C_{237}H_{345}N_{59}O_{72}S_2$	[338-368] [8)]	X	X	
67	873.2523	873.2510	6				X	
68	876.2488	876.2527	6	$C_{237}H_{347}N_{59}O_{73}S_2$	[338-368] [7,8)]		H	
69	870.5794	870.5846	6	$C_{237}H_{345}N_{59}O_{71}S_2$	[338-368]	X	X	
70	1162.8056	1162.8076	4	$C_{213}H_{307}N_{53}O_{61}S_2$	[338-368] [5)]		X	
71	930.4362	930.4476	5			X	X	
72	933.6405	933.6466	5	$C_{213}H_{307}N_{53}O_{62}S_2$	[338-368] [5,8)]	X		K351
73	951.4409	951.4462	4	$C_{170}H_{248}N_{44}O_{52}S_2$	[338-356]	X		
74	955.9403	955.9493	4	$C_{170}H_{250}N_{44}O_{53}S_2$	[338-356] [7)]		H	
75	955.4407	955.4449	4	$C_{170}H_{248}N_{44}O_{53}S_2$	[338-356] [8)]	X		
76	685.9835	685.9891	3	$C_{91}H_{134}N_{26}O_{25}S_2$	[350-356] [5)]	X		
77	691.3156	691.3213	3	$C_{91}H_{134}N_{26}O_{26}S_2$	[350-356] [5,8)]	X		

78	846.8000	846.8035	5	$C_{189}H_{281}N_{49}O_{56}S_3$	[352-372]	X	X	K368
79	1058.2454	1058.2531	4				X	
80	850.004	850.0024	5	$C_{189}H_{281}N_{49}O_{57}S_3$	[352-372] [8)]	X	X	
81	732.7431	732.7510	5	$C_{165}H_{243}N_{43}O_{46}S_3$	[352-372] [5)]		X	
82	590.2802	590.2808	5	$C_{124}H_{199}N_{35}O_{42}S_3$	[369-380]	X	X	K372
83	737.5990	737.5991	4			X	X	
84	983.1236	983.1303	3				X	
85	593.8726	593.8834	5	$C_{124}H_{201}N_{35}O_{43}S_3$	[369-380] [7)]		H	
86	741.598	741.5978	4	$C_{124}H_{199}N_{35}O_{43}S_3$	[369-380] [8)]	X	X	
87	593.4800	593.4797	5			X	X	
88	741.598	741.5978	4		[369-380] [8)]	X	X	
89	593.4800	593.4797	5				X	
90	596.6747	596.6793	5	$C_{124}H_{199}N_{35}O_{44}S_3$	[369-380] [8)]		X	
91	793.0405	793.0420	3	$C_{100}H_{161}N_{29}O_{32}S_3$	[369-380] [5)]		X	
92	595.0266	595.0334	4			X	X	
93	599.0262	599.0322	4	$C_{100}H_{161}N_{29}O_{33}S_3$	[369-380] [5, 8]	X	X	
94	618.7845	618.7925	4	$C_{104}H_{162}N_{30}O_{38}S_1$	[375-382]		X	K380
95	634.6263	634.6318	3	$C_{80}H_{124}N_{24}O_{28}S_1$	[375-382] [5)]	X		
96	710.6632	710.6689	3	$C_{90}H_{140}N_{26}O_{32}S_1$	[373-382] [5)]	X	X	
97	900.7518	900.7578	3	$C_{114}H_{178}N_{32}O_{42}S_1$	[373-382]		X	
98	675.8142	675.8197	4			X	X	
99	852.7515	852.7520	3	$C_{110}H_{174}N_{30}O_{38}S_1$	[407-415]		X	K407
100	639.8106	639.8154	4			X	X	
101	662.6586	662.6631	3	$C_{86}H_{136}N_{24}O_{28}S_1$	[407-415] [5)]	X	X	
102	619.4785	619.4837	6	$C_{160}H_{255}N_{49}O_{51}S_1$	[408-426]	X	X	K415
103	531.1240	531.1299	7			X		
104	575.6627	575.6680	5	$C_{122}H_{184}N_{36}O_{43}S_1$	[441-450]	X	X	K445
105	719.3277	719.3333	4			X	X	
106	579.2631	579.2707	5	$C_{122}H_{186}N_{36}O_{44}S_1$	[441-450] [7)]		H	
107	581.2634	581.2702	4	$C_{98}H_{148}N_{30}O_{34}S_1$	[441-450] [5,7)]		H	
108	768.6823	768.6869	3	$C_{98}H_{146}N_{30}O_{33}S_1$	[441-450] [5)]	X		
109	576.7616	576.7676	4			X		
110	671.3138	671.3145	4	$C_{108}H_{176}N_{36}O_{40}S_2$	[468-476] [6)]	X	X	K474
111	537.2528	537.2530	5			X	X	
112	704.6560	704.6624	3	$C_{84}H_{138}N_{30}O_{30}S_2$	[468-476] [6,5)]	X		
113	528.7429	528.7487	4			X		
114	568.0131	568.0183	4	$C_{92}H_{149}N_{29}O_{36}S_1$	[471-476]	X		
115	566.9285	566.9337	3	$C_{68}H_{111}N_{23}O_{26}S_1$	[471-476] [5)]	X		
116	598.5361	598.5422	4	$C_{98}H_{159}N_{33}O_{35}S_1$	[554-560]	X	X	K559
117	479.0289	479.0352	5			X	X	
118	455.9701	455.9760	4	$C_{74}H_{121}N_{27}O_{25}S_1$	[554-560] [5)]	X	X	

119	607.6264	607.6322	3			X	X	
120	425.2052	425.2104	4	$C_{72}H_{112}N_{24}O_{22}S_1$	[651-655] [5)]	X		K652
121	566.6069	566.6113	3			X		
122	567.7703	567.7767	4	$C_{96}H_{150}N_{30}O_{32}S_1$	[651-655]	X		
123	572.2781	572.2793	4	$C_{96}H_{152}N_{30}O_{33}S$	[651-655]] [7)]		H	
124	711.7656	711.7734	7	$C_{216}H_{331}N_{63}O_{67}S_3$	[653-681] [6)]		X	K668
125	777.8717	777.8749	4	$C_{135}H_{206}N_{40}O_{41}S_2$	[664-681] [5)]	X	X	
126	912.8345	912.8362	5	$C_{196}H_{303}N_{57}O_{63}S_3$	[656-681] [6)]		X	
127	760.8655	760.8648	6				X	
128	1040.8932	1040.8925	5	$C_{229}H_{343}N_{59}O_{76}S_2$	[682-717] [5)]		X	K690
129	1154.9458	1154.9454	5	$C_{253}H_{381}N_{65}O_{86}S_2$	[682-717]		X	
130	962.6211	962.6219	6			X	X	
131	1158.5446	1158.5475	5	$C_{253}H_{383}N_{65}O_{87}S_2$	[682-717] [7)]		H	
132	965.6205	965.6243	6				H	
133	646.0499	646.0560	4	$C_{107}H_{173}N_{31}O_{39}S_2$	[714-721]	X	X	K717
134	861.069	861.0728	3				X	
135	650.0489	650.0552	4	$C_{107}H_{173}N_{31}O_{40}S_2$	[714-721] [8)]	X	X	
136	670.9796	670.9844	3	$C_{83}H_{135}N_{25}O_{29}S_2$	[714-721] [5,8)]	X	X	
137	742.3402	742.3495	3	$C_{92}H_{149}N_{27}O_{33}S_2$	[717-721]		X	
138	557.0042	557.0142	4			X	X	
139	552.2560	552.2613	3	$C_{68}H_{111}N_{21}O_{23}S_2$	[717-721] [5)]	X		
140	1005.3302	1005.3360	6	$C_{260}H_{413}N_{75}O_{86}S_2$	[718-756]		X	K748
141	861.8522	861.8605	7				X	
142	864.1376	864.1456	7	$C_{260}H_{413}N_{75}O_{87}S_2$	[718-756] [8)]		X	
143	1001.4903	1001.4895	3	$C_{127}H_{204}N_{36}O_{46}S_1$	[739-756] [5)]		X	
144	751.1180	751.1231	4			X	X	
145	715.1474	715.1530	5	$C_{151}H_{243}N_{43}O_{55}S_1$	[739-756]	X	X	
146	893.6818	893.6893	4				X	
147	718.7489	718.7551	5	$C_{151}H_{245}N_{43}O_{56}S_1$	[739-756] [7)]		H	
148	1157.8936	1157.8990	3	$C_{146}H_{235}N_{43}O_{53}S_1$	[749-767]		X	K756
149	868.6730	868.6757	4			X	X	
150	695.1378	695.1420	5			X	X	
151	698.7365	698.7447	5	$C_{146}H_{237}N_{43}O_{54}S_1$	[749-767] [7)]		H	
152	730.6070	730.6126	4	$C_{122}H_{199}N_{37}O_{44}S_1$	[749-767] [5,7)]		H	
153	584.6856	584.6917	5				H	
154	967.8090	967.8107	3	$C_{122}H_{197}N_{37}O_{43}S_1$	[749-767] [5)]		X	
155	726.1093	726.1100	4				X	
156	631.7093	631.7181	5	$C_{134}H_{216}N_{40}O_{46}S_1$	[752-767]		X	
157	988.4799	988.4800	3	$C_{125}H_{203}N_{35}O_{44}S_2$	[757-770]		X	K767
158	741.612	741.6114	4			X	X	
159	593.4913	593.4905	5			X	X	

160	746.1049	746.1146	4	$C_{125}H_{205}N_{35}O_{45}S_2$	[757-770] [7)]		H	
161	993.8126	993.8126	3	$C_{125}H_{203}N_{35}O_{45}S_2$	[757-770] [8)]		X	
162	745.611	745.6101	4			X	X	
163	1197.0838	1197.0836	2	$C_{101}H_{165}N_{29}O_{34}S_2$	[757-770] [5)]		X	
164	798.3874	798.3917	3			X	X	
165	603.5399	603.5483	4	$C_{101}H_{167}N_{29}O_{35}S_2$	[757-770] [5,7)]		H	
166	902.0965	902.1010	3	$C_{114}H_{182}N_{32}O_{42}S_1$	[757-768]	X	X	
167	1067.5108	1067.5153	2	$C_{90}H_{144}N_{26}O_{32}S_1$	[757-768] [5)]	X		
168	712.0128	712.0132	3				X	
169	602.8903	602.8895	5	$C_{132}H_{200}N_{36}O_{41}S_2$	[768-778]	X	X	K770
170	753.3620	753.3601	4			X	X	
171	1004.1401	1004.1450	3				X	
172	757.8599	757.8633	4	$C_{132}H_{202}N_{36}O_{42}S_2$	[768-778] [7)]		H	
173	606.4879	606.4922	5				H	
174	1009.4764	1009.4760	3	$C_{132}H_{200}N_{36}O_{42}S_2$	[768-778] [8)]	X	X	
175	757.3602	757.3594	4				X	
176	606.0896	606.0891	5				X	
177	610.7901	610.7944	4	$C_{108}H_{162}N_{30}O_{31}S_2$	[768-778] [5)]	X	X	
178	814.0541	814.0566	3			X	X	
179	615.2913	615.2971	4	$C_{108}H_{164}N_{30}O_{32}S_2$	[768-778] [5,7)]		H	
180	819.3825	819.3882	3	$C_{108}H_{162}N_{30}O_{32}S_2$	[768-778] [5,8)]	X	X	
181	614.7876	614.7932	4			X	X	
182	674.5163	674.5215	6	$C_{175}H_{285}N_{53}O_{55}S_1$	[805-831]	X		K828
183	735.3577	735.3599	3	$C_{94}H_{150}N_{26}O_{33}S_1$	[827-831]	X	X	
184	551.7722	551.7718	4			X	X	
185	545.2670	545.2722	3	$C_{70}H_{112}N_{20}O_{23}S_1$	[827-831] [5)]	X	X	
186	583.0301	583.0370	4	$C_{99}H_{157}N_{29}O_{34}S_1$	[829-834]		X	K831
187	586.9534	586.9579	3	$C_{75}H_{119}N_{23}O_{24}S_1$	[829-834] [5)]	X	X	
188	771.4043	771.4114	4	$C_{132}H_{220}N_{42}O_{41}S_1$	[829-840]		X	
189	617.3209	617.3307	5				X	
190	514.6029	514.6102	6				X	
191	733.6799	733.6874	3	$C_{89}H_{147}N_{29}O_{34}S_1$	[840-844]		X	K840
192	550.5169	550.5169	4				X	
193	668.6802	668.6787	6	$C_{169}H_{284}N_{50}O_{58}S_2$	[841-861]		X	K855
194	642.831	642.8298	4	$C_{109}H_{182}N_{30}O_{39}S_1$	[856-864]	X	X	K861
195	856.7718	856.7706	3			X	X	
196	647.3260	647.3330	4	$C_{109}H_{184}N_{30}O_{40}S_1$	[856-864] [7)]		H	
197	893.4140	893.4193	4	$C_{152}H_{232}N_{44}O_{54}S_1$	[862-880]	X	X	K864
198	714.9320	714.9369	5			X	X	
199	718.5317	718.5396	5	$C_{152}H_{234}N_{44}O_{55}S_1$	[862-880] [7)]		H	
200	750.8456	750.8536	4	$C_{128}H_{194}N_{38}O_{44}S_1$	[862-880] [5)]		X	

201	989.4524	989.4512	4	$C_{171}H_{252}N_{48}O_{57}S_2$	[865-886] [6)]		X	K880
202	1060.9844	1060.9923	4	$C_{183}H_{274}N_{52}O_{61}S_2$	[865-889] [6)]		X	
203	848.9908	848.9954	5			X	X	
204	852.5901	852.5975	5	$C_{183}H_{276}N_{52}O_{62}S_2$	[865-889] [6,7)]		H	
205	710.6585	710.6659	6				H	
206	738.5376	738.5445	5	$C_{159}H_{238}N_{46}O_{52}S_2$	[865-889] [6,5,7)]		H	
207	1224.2280	1224.2322	3	$C_{159}H_{236}N_{46}O_{51}S_2$	[865-889] [6, 5)]		X	
208	918.4220	918.4260	4			X	X	
209	690.066	690.0706	4	$C_{116}H_{181}N_{33}O_{41}S_2$	[881-890]	X	X	K889
210	729.6655	729.6707	3	$C_{92}H_{143}N_{27}O_{31}S_2$	[881-890] [5)]	X	X	
211	694.5670	694.5738	4	$C_{116}H_{183}N_{33}O_{42}S_2$	[881-890] [7)]		H	
212	882.5682	882.5748	6	$C_{236}H_{337}N_{61}O_{77}S_1$	[919-955] [5)]	X		K945
213	977.6133	977.6190	6	$C_{260}H_{375}N_{67}O_{87}S_1$	[919-955]	X	X	
214	1172.9337	1172.9418	5				X	
215	1066.7587	1066.7583	4	$C_{181}H_{279}N_{55}O_{63}S_1$	[956-978]		X	K969
216	853.6026	853.6086	5			X		
217	711.5028	711.5079	6			X	X	
218	609.9998	610.0084	7				X	
219	714.5037	714.5103	6	$C_{181}H_{281}N_{55}O_{64}S_1$	[956-978] [7)]		H	
220	616.4599	616.4644	6	$C_{157}H_{241}N_{49}O_{53}S_1$	[956-978] [5)]	X		
221	739.5514	739.5556	5				X	
222	743.1513	743.1577	5	$C_{157}H_{243}N_{49}O_{54}S_1$	[956-978] [5,7)]		H	
223	618.7838	618.7924	6	$C_{158}H_{239}N_{47}O_{55}S_1$	[956-973]		X	
224	742.3406	742.3487	5			X	X	
225	927.6770	927.6846	4				X	
226	870.8224	870.8278	5	$C_{188}H_{293}N_{53}O_{64}S_1$	[970-993]	X	X	K978
227	725.8507	725.8582	6				X	
228	945.7093	945.7172	4	$C_{164}H_{255}N_{47}O_{54}S_1$	[970-993] [5)]		X	
229	778.9748	778.9789	5	$C_{170}H_{260}N_{46}O_{57}S_1$	[974-993]	X	X	
230	973.4654	973.4724	4				X	
231	830.9014	830.9061	4	$C_{146}H_{222}N_{40}O_{47}S_1$	[974-993] [5)]	X		
232	962.7864	962.7906	3	$C_{122}H_{192}N_{34}O_{45}S_1$	[974-984]	X	X	
233	772.6981	772.7029	3	$C_{98}H_{154}N_{28}O_{35}S_1$	[974-984] [5)]	X	X	
234	840.1704	840.1750	4	$C_{148}H_{233}N_{39}O_{48}S_1$	[985-1000]	X		K993
235	786.6422	786.6493	4	$C_{141}H_{215}N_{39}O_{41}S_1$	[1052-1063]		X	K1061
236	809.6231	809.6287	4	$C_{133}H_{215}N_{41}O_{47}S_3$	[1064-1078] [6)]	X	X	K1065
237	813.6219	813.6274	4	$C_{133}H_{215}N_{41}O_{48}S_3$	[1064-1078] [6,8)]	X	X	
238	889.0747	889.0814	3	$C_{109}H_{177}N_{35}O_{37}S_3$	[1064-1078] [6,5)]	X	X	
239	945.2021	945.2061	4	$C_{161}H_{253}N_{45}O_{58}S_1$	[1079-1098]	X	X	K1097
240	922.9169	922.9217	4	$C_{164}H_{234}N_{42}O_{54}S_1$	[1099-1115]	X	X	K1109
241	1040.1314	1040.1387	3	$C_{140}H_{196}N_{36}O_{44}S_1$	[1099-1115] [5)]	X	X	

242	955.1780	955.1823	4	$C_{169}H_{241}N_{43}O_{57}S_1$	[1098-1115]	X		
243	1083.1485	1083.1523	3	$C_{145}H_{203}N_{37}O_{47}S_1$	[1098-1115] [5)]	X		
244	1128.9239	1128.9299	5	$C_{251}H_{367}N_{63}O_{84}S_1$	[1097-1130]		X	
245	1268.3416	1268.3442	4	$C_{227}H_{329}N_{57}O_{74}S_1$	[1097-1131] [5)]	X		
246	568.0434	568.0428	4	$C_{96}H_{161}N_{27}O_{34}S_1$	[1132-1137]	X	X	
247	572.5384	572.5460	4	$C_{96}H_{163}N_{27}O_{35}S_1$	[1132-1137] [7)]		H	
248	458.2307	458.2383	5				H	K1132
249	572.9630	572.9703	3	$C_{72}H_{125}N_{21}O_{25}S_1$	[1132-1137] [5,7)]		H	
250	566.9621	566.9663	3	$C_{72}H_{123}N_{21}O_{24}S_1$	[1132-1137] [5)]	X	X	
251	657.5689	657.5737	4	$C_{108}H_{179}N_{33}O_{41}S_1$	[1133-1141]		X	K1137
252	683.9344	683.9406	5	$C_{152}H_{231}N_{41}O_{47}S_1$	[1138-1153]	X	X	
253	854.6695	854.6740	4			X	X	
254	859.1713	859.1771	4	$C_{152}H_{233}N_{41}O_{48}S_1$	[1138-1153] [7)]		H	
255	687.5370	687.5433	5				H	K1152
256	573.1142	573.1207	6				H	
257	712.1029	712.1083	4	$C_{128}H_{193}N_{35}O_{37}S_1$	[1138-1153] [5)]	X		
258	733.1138	733.1193	4	$C_{134}H_{201}N_{33}O_{39}S_1$	[1142-1153]	X	X	
259	553.6184	553.6230	3	$C_{69}H_{119}N_{21}O_{24}S_1$	[1153-1158] [5)]	X	X	
260	562.5303	562.5381	4	$C_{93}H_{159}N_{27}O_{35}S_1$	[1153-1158] [7)]		H	K1153
261	450.2242	450.2321	5				H	
262	1233.7552	1233.7631	5	$C_{268}H_{399}N_{71}O_{89}S_4$	[1154-1192] [6)]		X	K1158
263	1028.2960	1028.3038	6				X	
264	981.4701	981.4788	3	$C_{126}H_{200}N_{34}O_{45}S_1$	[1193-1203]		X	
265	736.361	736.3605	4			X	X	
266	589.2900	589.2899	5			X	X	
267	598.2896	598.2974	4	$C_{102}H_{164}N_{28}O_{36}S_1$	[1193-1203] [5,7)]		H	K1198
268	740.8566	740.8636	4	$C_{126}H_{202}N_{34}O_{46}S_1$	[1193-1203] [7)]		H	
269	592.8851	592.8925	5				H	
270	791.3863	791.3904	3	$C_{102}H_{162}N_{28}O_{35}S_1$	[1193-1203] [5)]	X	X	
271	569.9479	569.9543	3	$C_{72}H_{118}N_{22}O_{24}S_1$	[1202-1207] [5)]	X	X	
272	570.2786	570.2843	4	$C_{96}H_{156}N_{28}O_{34}S_1$	[1202-1207]	X	X	
273	661.5712	661.5762	4	$C_{112}H_{179}N_{33}O_{39}S_1$	[1199-1207]		X	
274	529.4550	529.4630	5			X	X	
275	519.0027	519.0106	4	$C_{88}H_{141}N_{27}O_{29}S_1$	[1199-1207] [5)]	X	X	K1203
276	752.3671	752.3655	5	$C_{170}H_{249}N_{43}O_{52}S_1$	[1199-1220] [5)]		X	
277	866.4133	866.4185	5	$C_{194}H_{287}N_{49}O_{62}S_1$	[1199-1220]		X	
278	722.1778	722.1833	6			X	X	
279	619.1523	619.1583	7			X		
280	1069.5106	1069.5145	4	$C_{191}H_{284}N_{48}O_{62}S_1$	[1204-1226]		X	
281	855.8153	855.8126	5			X	X	K1220
282	713.3400	713.3450	6			X	X	

283	1235.5961	1235.5951	3	$C_{167}H_{246}N_{42}O_{52}S_1$	[1204-1226] [5)]		X	
284	926.9425	926.9482	4			X	X	
285	716.3395	716.3474	6	$C_{191}H_{286}N_{48}O_{63}S_1$	[1204-1226] [7)]		H	
286	859.4074	859.4153	5				H	
287	724.7014	724.7094	3	$C_{95}H_{154}N_{26}O_{30}S_1$	[1216-1226] [5)]		X	
288	596.0538	596.0587	4	$C_{101}H_{169}N_{29}O_{35}S_1$	[1219-1226]	X	X	
289	604.3158	604.3209	3	$C_{77}H_{131}N_{23}O_{25}S_1$	[1219-1226] [5)]	X	X	
290	661.5776	661.5831	4	$C_{114}H_{183}N_{31}O_{39}S_1$	[1221-1230]	X	X	K1226
291	691.6829	691.6865	3	$C_{90}H_{145}N_{25}O_{29}S_1$	[1221-1230] [5)]	X	X	
292	1045.1789	1045.1838	3	$C_{135}H_{213}N_{39}O_{45}S_1$	[1227-1239]	X	X	K1230
293	784.1342	784.1397	4			X	X	
294	627.5074	627.5132	5			X	X	
295	855.0922	855.0961	3	$C_{111}H_{175}N_{33}O_{35}S_1$	[1227-1239] [5)]	X	X	
296	641.5682	641.5735	4			X	X	
297	551.7740	551.7817	10	$C_{237}H_{375}N_{73}O_{77}S_1$	[1227-1260]		X	
298	612.9710	612.9789	9				X	
299	689.4657	689.4752	8				X	
300	787.8270	787.8271	7			X	X	
301	918.9559	918.9644	6				X	
302	706.3595	706.3613	7	$C_{213}H_{337}N_{67}O_{67}S_1$	[1227-1260] [5)]		X	
303	618.1919	618.1921	8				X	
304	646.0688	646.0767	4	$C_{111}H_{177}N_{33}O_{36}S$	[1227-1239] [5,7)]		H	
305	517.0551	517.0629	5				H	
306	788.6351	788.6429	4	$C_{135}H_{215}N_{39}O_{46}S$	[1227-1239] [7)]		H	
307	631.1081	631.1159	5				H	
308	526.0901	526.0979	6				H	
309	620.4356	620.4434	8	$C_{213}H_{339}N_{67}O_{68}S_1$	[1227-1260] [5,7)]		H	
310	614.9726	614.9800	9	$C_{237}H_{377}N_{73}O_{78}S_1$	[1227-1260] [7)]		H	
311	821.4076	821.4122	4	$C_{137}H_{228}N_{40}O_{51}S_1$	[1260-1274]	X	X	K1260
312	904.7876	904.7922	3	$C_{113}H_{190}N_{34}O_{41}S_1$	[1260-1274] [5)]	X	X	
313	660.9260	660.9339	5	$C_{137}H_{230}N_{40}O_{52}S$	[1260-1274] [7)]		H	
314	1019.2111	1019.2093	3	$C_{135}H_{223}N_{35}O_{43}S_1$	[1322-1334]	X	X	K1333
315	764.6542	764.6593	4				X	
316	829.1136	829.1215	3	$C_{111}H_{185}N_{29}O_{33}S_1$	[1322-1334] [5)]		X	
317	752.0474	752.0553	3	$C_{95}H_{160}N_{28}O_{33}S_1$	[1329-1334]		X	
318	564.2878	564.2934	4			X	X	
319	561.9631	561.9664	3	$C_{95}H_{160}N_{28}O_{33}S_1$	[1329-1334] [5)]	X		
320	615.5233	615.5311	5	$C_{135}H_{225}N_{35}O_{44}S$	[1322-1334] [7)]		H	
321	926.0926	926.1015	3	$C_{120}H_{182}N_{32}O_{42}S_1$	[1334-1344]		X	K1334
322	805.6307	805.6346	4	$C_{141}H_{211}N_{39}O_{46}S_1$	[1335-1348]	X	X	K1347
323	550.1286	550.1368	8	$C_{187}H_{281}N_{59}O_{63}S_1$	[1366-1388]		X	K1378

324	638.1296	638.1351	6	$C_{163}H_{243}N_{53}O_{53}S_1$	[1366-1388] [5)]	X		
325	665.3010	665.3088	4	$C_{112}H_{168}N_{36}O_{38}S_1$	[1371-1384] [5)]		X	
326	915.0206	915.0264	5	$C_{201}H_{296}N_{54}O_{65}S_2$	[1435-1460]	X	X	K1436
327	762.6899	762.6899	6			X	X	
328	804.5682	804.5761	5	$C_{177}H_{260}N_{48}O_{56}S_2$	[1435-1460] [5,7)]		H	
329	918.6212	918.6291	5	$C_{201}H_{298}N_{54}O_{66}S_2$	[1435-1460] [7)]		H	
330	800.9677	800.9734	5	$C_{177}H_{258}N_{48}O_{55}S_2$	[1435-1460] [5)]	X	X	
331	1000.9573	1000.9655	4			X	X	
332	918.2202	918.2254	5	$C_{201}H_{296}N_{54}O_{66}S_2$	[1435-1460] [8)]	X	X	
333	765.3635	765.3557	6			X		
334	572.5379	572.5367	4	$C_{96}H_{155}N_{31}O_{32}S_1$	[1473-1477]	X	X	K1473
335	458.2304	458.2308	5			X	X	
336	572.9528	572.9578	3	$C_{72}H_{117}N_{25}O_{22}S_1$	[1473-1477] [5)]	X		
337	429.9649	429.9710	4			X		
338	747.6392	747.6392	7	$C_{219}H_{344}N_{66}O_{77}S_3$	[1474-1504] [6)]		X	K1495
339	872.0774	872.0771	6			X	X	
340	932.2377	932.2387	5	$C_{195}H_{306}N_{60}O_{67}S_3$	[1474-1504] [6, 5)]		X	
341	777.0347	777.0336	6				X	
342	931.8216	931.8275	5	$C_{193}H_{304}N_{56}O_{72}S_3$	[1478-1504] [6)]	X		
343	1046.7570	1046.76	7	$C_{314}H_{463}N_{89}O_{111}S_2$	[1496-1544]	X	X	K1504
344	814.3652	814.3718	9				X	
345	766.3659	766.3738	3	$C_{92}H_{153}N_{33}O_{34}S$	[1544-1548] [7)]		H	K1544
346	823.7555	823.7605	3	$C_{105}H_{177}N_{29}O_{37}S_1$	[1605-1612]		X	K1609
347	618.0715	618.0718	4			X	X	
348	950.0033	950.0044	2	$C_{81}H_{139}N_{23}O_{27}S_1$	[1605-1612] [5)]		X	
349	633.6669	633.6722	3			X	X	
350	639.6679	639.6657	3	$C_{81}H_{141}N_{23}O_{28}S_1$	[1605-1612] [5,7)]		H	
351	622.5671	622.5750	4	$C_{105}H_{179}N_{29}O_{38}S$	[1605-1612] [7)]		H	
352	653.3223	653.3270	3	$C_{81}H_{136}N_{24}O_{30}S_1$	[1669-1676] [5)]	X		K1669
353	632.8130	632.8139	4	$C_{105}H_{174}N_{30}O_{40}S_1$	[1669-1676]	X	X	
354	671.3490	671.3491	5	$C_{141}H_{238}N_{42}O_{50}S_1$	[1670-1684]	X	X	K1676
355	838.9298	838.9351	4				X	
356	1118.2451	1118.2437	3			X	X	
357	696.3640	696.3689	4	$C_{117}H_{200}N_{36}O_{40}S_1$	[1670-1684] [5)]	X	X	
358	852.7502	852.7501	3	$C_{105}H_{174}N_{32}O_{40}S_1$	[1670-1677]	X	X	
359	639.8146	639.8144	4			X	X	
360	662.6572	662.6618	3	$C_{81}H_{136}N_{26}O_{30}S_1$	[1670-1677] [5)]	X		
361	588.0424	588.0499	4	$C_{101}H_{165}N_{27}O_{35}S$	[1670-1677] [7)]		H	
362	843.4299	843.4378	4	$C_{141}H_{240}N_{42}O_{51}S_1$	[1670-1684] [7)]		H	
363	674.9439	674.9518	5				H	
364	800.4025	800.4122	4	$C_{134}H_{228}N_{40}O_{46}S_1$	[1677-1690]	X	X	K1684

365	640.531	640.5308	5			X	X	
366	657.8470	657.8459	4	$C_{110}H_{190}N_{34}O_{36}S_1$	[1677-1690] [5)]		X	
367	921.4351	921.4404	5	$C_{197}H_{304}N_{58}O_{66}S_2$	[1691-1719] [6)]	X	X	K1718
368	768.0292	768.0349	6			X	X	
369	807.3816	807.3879	5	$C_{173}H_{266}N_{52}O_{56}S_2$	[1691-1719] [6, 5)]	X		
370	748.8686	748.8772	4	$C_{136}H_{202}N_{38}O_{37}S_1$	[1747-1763] [5)]		X	K1747
371	713.3496	713.3566	5	$C_{160}H_{240}N_{44}O_{47}S_1$	[1747-1763]	X	X	
372	891.4396	891.4444	4				X	
373	753.3730	753.3808	4	$C_{136}H_{204}N_{38}O_{38}S$	[1747-1763] [5,7)]		H	
374	602.8984	602.9062	5				H	
375	716.9513	716.9592	5	$C_{160}H_{242}N_{44}O_{48}S$	[1747-1763] [7)]		X	
376	983.7432	983.7432	8	$C_{351}H_{535}N_{93}O_{111}S_1$	[1748-1803]		X	K1792
377	874.5323	874.5504	9				X	
378	1042.5166	1042.5243	7	$C_{327}H_{497}N_{87}O_{101}S_1$	[1748-1803] [5)]	X	X	
379	788.5763	788.5831	5	$C_{171}H_{264}N_{46}O_{59}S_1$	[1783-1803]	X	X	
380	985.4701	985.4777	4				X	
381	842.9059	842.9108	4	$C_{153}H_{238}N_{44}O_{50}S_1$	[1783-1803] [5)]	X		
382	757.3567	757.3622	4	$C_{127}H_{200}N_{38}O_{46}S_1$	[1793-1804]	X	X	K1803
383	606.0854	606.0912	5			X	X	
384	614.7904	614.7960	4	$C_{103}H_{162}N_{32}O_{36}S_1$	[1793-1804] [5)]	X	X	
385	485.2308	485.2366	4	$C_{78}H_{128}N_{28}O_{28}S_1$	[1797-1894] [5)]	X		
386	502.4345	502.4443	5	$C_{102}H_{166}N_{34}O_{38}S_1$	[1797-1894]	X	X	
387	711.3338	711.3401	4	$C_{126}H_{184}N_{36}O_{38}S_1$	[1811-1825] [5)]	X	X	K1817
388	853.9001	853.9058	4	$C_{150}H_{222}N_{42}O_{48}S_1$	[1811-1825]	X		
389	600.9977	601.0028	7	$C_{186}H_{274}N_{50}O_{60}S_1$	[1911-1933]	X	X	K1914
390	700.9961	701.0020	6			X	X	
391	840.9955	841.0008	5			X	X	
392	1050.9944	1050.9990	4			X	X	
393	908.4240	908.4327	4	$C_{162}H_{234}N_{42}O_{52}S_1$	[1911-1933] [5)]	X	X	
394	726.9420	726.9478	5			X	X	
395	761.4938	761.4997	7	$C_{237}H_{343}N_{61}O_{78}S_1$	[1911-1942]		X	
396	888.2435	888.2484	6			X	X	
397	1065.6906	1065.6967	5			X	X	
398	1331.8702	1331.8690	4			X		
399	793.2019	793.2048	6	$C_{213}H_{305}N_{55}O_{68}S_1$	[1911-1942] [5)]	X	X	
400	951.6411	951.6442	5			X	X	
401	730.5455	730.5499	5	$C_{162}H_{238}N_{44}O_{51}S_1$	[1911-1933] [5,7)]		H	
402	608.9525	608.9595	6				H	
403	844.5950	844.6029	5	$C_{186}H_{276}N_{50}O_{61}S_1$	[1911-1933] [7)]		H	
404	703.9959	704.0037	6				H	
405	603.5682	603.5757	7				H	

406	955.2385	955.2463	5	$C_{213}H_{307}N_{55}O_{69}S_1$	[1911-1942] [5,7)]		H	
407	796.1987	796.2066	6				H	
408	1069.2914	1069.2993	5	$C_{237}H_{345}N_{61}O_{79}S_1$	[1911-1942] [7)]		H	
409	891.2429	891.2507	6				H	
410	764.0661	764.0732	7				H	
411	668.6835	668.6900	8				H	
412	815.0279	815.0357	6	$C_{216}H_{306}N_{56}O_{73}S_1$	[1915-1942]		X	K1933
413	863.7853	863.7833	5	$C_{192}H_{268}N_{50}O_{63}S_1$	[1915-1942] [5)]	X		
414	1123.2422	1123.2466	4	$C_{192}H_{285}N_{51}O_{68}S_3$	[1995-2020] [6)]	X	X	K2012
415	1307.2352	1307.2386	3	$C_{168}H_{247}N_{45}O_{58}S_3$	[1995-2020] [6,5)]	X	X	
416	980.6818	980.6809	4				X	
417	1312.5663	1312.5703	3	$C_{168}H_{247}N_{45}O_{59}S_3$	[1995-2020] [6,5,8)]	X		
418	687.5645	687.5693	4	$C_{118}H_{179}N_{33}O_{39}S_2$	[2012-2020]	X		
419	795.0286	795.0339	3	$C_{102}H_{155}N_{27}O_{37}S_1$	[2001-2013] [5)]	X		
420	1192.0433	1192.0471	2			X		
421	1313.2343	1313.2422	3	$C_{168}H_{249}N_{45}O_{59}S_3$	[1995-2020] [5,7)]		H	
422	985.1757	985.1835	4				H	
423	902.3935	902.4014	5	$C_{192}H_{287}N_{51}O_{69}S_3$	[1995-2020] [7)]		H	
424	768.1187	768.1235	4	$C_{133}H_{209}N_{33}O_{48}S_1$	[2021-2032]	X	X	K2023
425	833.7379	833.7406	3	$C_{109}H_{171}N_{27}O_{38}S_1$	[2021-2032] [5)]	X		
426	795.6244	795.6301	4	$C_{133}H_{215}N_{37}O_{49}S_2$	[2024-2036]	X	X	K2032
427	1060.5025	1060.5049	3				X	
428	799.6214	799.6293	4	$C_{133}H_{215}N_{37}O_{50}S_2$	[2024-2036] [8)]		X	
429	870.4122	870.4160	3	$C_{109}H_{177}N_{31}O_{39}S_2$	[2024-2036] [5)]	X	X	
430	640.3106	640.3139	4	$C_{105}H_{176}N_{32}O_{38}S_2$	[2029-2036]	X	X	
431	663.3236	663.3278	3	$C_{81}H_{138}N_{26}O_{28}S_2$	[2029-2036] [5)]	X	X	
432	621.0475	621.0463	4	$C_{101}H_{165}N_{33}O_{36}S_2$	[2032-2038]		X	
433	657.5592	657.5670	4	$C_{109}H_{179}N_{31}O_{40}S_2$	[2024-2036] [5)]		X	
434	800.1254	800.1332	4	$C_{133}H_{217}N_{37}O_{50}S_2$	[2024-2036] [5,7)]		H	
435	640.3003	640.3082	5				H	
436	1223.3406	1223.3533	4	$C_{213}H_{333}N_{57}O_{73}S_1$	[2095-2127]		X	K2100
437	978.8777	978.8836	5			X	X	
438	769.7049	769.7112	6	$C_{208}H_{306}N_{56}O_{62}S_1$	[2164-2189]	X	X	K2177
439	923.4463	923.4520	5			X	X	
440	608.4424	608.4426	7	$C_{190}H_{282}N_{52}O_{58}S_1$	[2178-2198]		X	K2189
441	709.6754	709.6818	6			X	X	
442	851.4121	851.4166	5			X	X	
443	669.3197	669.3249	6	$C_{180}H_{264}N_{48}O_{55}S_1$	[2178-2196]	X		
444	860.9156	860.9180	4	$C_{156}H_{226}N_{42}O_{45}S_1$	[2178-2196] [5)]		X	
445	688.9298	688.9354	5			X	X	
446	640.3123	640.3174	4	$C_{112}H_{172}N_{32}O_{35}S_1$	[2178-2190] [5)]	X		

447	686.0792	686.0838	4	$C_{116}H_{185}N_{35}O_{38}S_2$	[2197-2206]	X	X	K2198
448	690.0788	690.0831	4	$C_{116}H_{185}N_{35}O_{39}S_2$	[2197-2206] [8)]	X	X	
449	729.6816	729.6865	3	$C_{92}H_{147}N_{29}O_{29}S_2$	[2197-2206] [5,8)]	X		
450	724.3543	724.3543	3	$C_{92}H_{147}N_{29}O_{28}S_2$	[2197-2206] [5)]	X	X	
451	548.0129	548.0208	4	$C_{92}H_{149}N_{29}O_{29}S_2$	[2197-2206] [5,7)]		H	
452	690.5792	690.5870	4	$C_{116}H_{187}N_{35}O_{39}S_2$	[2197-2206] [7)]		H	
453	552.6633	552.6711	5				H	
454	694.5779	694.5858	4	$C_{116}H_{187}N_{35}O_{40}S_2$	[2197-2206] [7,8)]		H	
455	555.8623	555.8701	5				H	
456	771.1319	771.1357	4	$C_{135}H_{209}N_{39}O_{42}S_1$	[2297-2308]	X	X	K2307
457	1027.8387	1027.8457	3				X	
458	837.7528	837.7569	3	$C_{111}H_{171}N_{33}O_{32}S_1$	[2297-2308] [5)]	X		
459	633.0648	633.0727	4	$C_{111}H_{173}N_{33}O_{33}S$	[2297-2308] [5,7)]		H	
460	775.6311	775.6389	4	$C_{135}H_{211}N_{39}O_{43}S$	[2297-2308] [7)]		H	
461	620.7048	620.7127	5				H	
462	681.3348	681.3368	4	$C_{117}H_{184}N_{34}O_{39}S_1$	[2341-2350]		X	K2341
463	545.271	545.2709	5			X	X	
464	538.7654	538.7711	4	$C_{93}H_{146}N_{28}O_{29}S_1$	[2341-2350] [5)]	X	X	
465	872.9209	872.9280	4	$C_{154}H_{234}N_{42}O_{49}S_1$	[2336-2351]	X	X	K2350
466	698.5386	698.5444	5				X	
467	702.1387	702.1465	5	$C_{154}H_{236}N_{42}O_{50}S$	[2342-2357] [7)]		H	
468	1177.5658	1177.5736	4	$C_{205}H_{320}N_{54}O_{69}S_2$	[2351-2376]		X	K2373
469	942.2552	942.2605	5				X	
470	785.3799	785.3850	6				X	
471	763.3593	763.3685	5	$C_{162}H_{258}N_{44}O_{58}S_2$	[2358-2376]		X	
472	795.0334	795.0388	3	$C_{98}H_{159}N_{29}O_{36}S_2$	[2363-2374] [5,8)]	X		
473	735.0918	735.0984	4	$C_{122}H_{197}N_{35}O_{45}S_2$	[2363-2374]	X		
474	695.9886	695.9973	3	$C_{86}H_{140}N_{24}O_{34}S_1$	[2371-2374]		X	
475	945.8584	945.8626	5	$C_{205}H_{322}N_{54}O_{70}S_2$	[2351-2376] [7)]		H	
476	788.3812	788.3868	6				H	
477	831.5651	831.5729	6	$C_{215}H_{339}N_{57}O_{75}S_2$	[2351-2378] [7,8)]		H	
478	550.7694	550.7692	4	$C_{91}H_{150}N_{26}O_{35}S_1$	[2374-2378]	X		K2376
479	518.5057	518.5091	4	$C_{86}H_{143}N_{25}O_{32}S_1$	[2375-2378]		X	
480	555.2646	555.2724	4	$C_{91}H_{152}N_{26}O_{36}S$	[2374-2378] [7)]		H	
481	622.5489	622.5503	4	$C_{102}H_{163}N_{35}O_{36}S_1$	[2377-2383]	X	X	K2378
482	498.2405	498.2417	5			X	X	
483	870.8114	870.8119	5	$C_{189}H_{285}N_{55}O_{58}S_3$	[2406-2434] [5,6)]	X		K2423
484	820.8884	820.8882	6	$C_{213}H_{323}N_{61}O_{68}S_3$	[2406-2434] [6)]	X	X	
485	907.2075	907.2154	5	$C_{192}H_{291}N_{57}O_{65}S_3$	[2406-2431] [6)]		X	
486	756.17295	756.1808	6				X	
487	760.8677	760.8616	4	$C_{133}H_{202}N_{36}O_{44}S_1$	[2432-2443]		X	K2434

488	814.9004	814.9055	4	$C_{136}H_{226}N_{38}O_{52}S_1$	[2506-2520]	X	X	K2506
489	655.7207	655.7285	5	$C_{136}H_{228}N_{38}O_{53}S$	[2506-2520] [7)]		H	
490	901.0845	901.0895	3	$C_{113}H_{177}N_{33}O_{42}S_1$	[2632-2640]		X	K2633
491	676.0688	676.0685	4			X	X	
492	541.0452	541.0563	5				X	
493	710.9965	711.0006	3	$C_{89}H_{139}N_{27}O_{32}S_1$	[2632-2640] [5)]	X	X	
494	776.8408	776.8596	4	$C_{135}H_{198}N_{38}O_{45}S_1$	[2632-2648] [5)]		X	
495	735.7323	735.7421	5	$C_{159}H_{236}N_{44}O_{55}S_1$	[2632-2648]	X	X	
496	919.4194	919.4264	4				X	
497	537.9976	538.0045	4	$C_{89}H_{141}N_{27}O_{33}S_1$	[2632-2640] [5,7)]		H	
498	680.5639	680.5717	4	$C_{113}H_{179}N_{33}O_{43}S_1$	[2632-2640] [7)]		H	
499	544.6511	544.6589	5				H	
500	694.9178	694.9235	5	$C_{144}H_{228}N_{44}O_{50}S_3$	[2719-2734] [6)]	X		K2733
501	725.8292	725.8369	4	$C_{120}H_{190}N_{38}O_{40}S_3$	[2719-2734] [6, 5)]	X	X	
502	581.9518	581.9597	3	$C_{71}H_{122}N_{24}O_{23}S_2$	[2729-2734] [5)]		X	
503	726.7763	726.7827	7	$C_{221}H_{334}N_{66}O_{71}S_1$	[2734-2763]		X	K2754
504	726.6769	726.6848	6	$C_{191}H_{284}N_{56}O_{60}S_1$	[2735-2763] [5)]		X	
505	633.0611	633.0606	4	$C_{108}H_{173}N_{31}O_{35}S_2$	[2773-2780]	X	X	K2779
506	843.7501	843.7462	3				X	
507	637.0525	637.0604	4	$C_{108}H_{173}N_{31}O_{36}S_2$	[2773-2780] [8)]		X	
508	653.6531	653.6573	3	$C_{84}H_{135}N_{25}O_{25}S_2$	[2773-2780] [5)]	X	X	
509	649.0696	649.0695	4	$C_{109}H_{177}N_{31}O_{40}S_1$	[2780-2787]	X	X	K2780
510	741.6782	741.6836	3	$C_{92}H_{147}N_{27}O_{35}S_1$	[2780-2784]	X	X	
511	556.5066	556.5146	4			X	X	
512	551.5897	551.5953	3	$C_{68}H_{109}N_{21}O_{25}S_1$	[2780-2784] [5)]	X		
513	570.6890	570.6868	5	$C_{120}H_{197}N_{35}O_{43}S_1$	[2780-2789]	X	X	K2787
514	713.1091	713.1079	4			X	X	
515	570.5374	570.5422	4	$C_{96}H_{159}N_{29}O_{33}S_1$	[2780-2789] [5)]	X	X	
516	907.7743	907.7765	3	$C_{114}H_{185}N_{33}O_{42}S_1$	[2781-2789]	X	X	
517	681.084	681.0842	4			X	X	
518	545.0617	545.0693	5				X	
519	717.6835	717.6887	3	$C_{90}H_{147}N_{27}O_{32}S_1$	[2781-2789] [5)]	X	X	
520	554.0216	554.0276	4	$C_{92}H_{153}N_{27}O_{34}S_1$	[2785-2789]	X	X	
521	548.2741	548.2793	3	$C_{68}H_{115}N_{21}O_{24}S_1$	[2785-2789] [5)]	X	X	
522	574.2838	574.2902	5	$C_{120}H_{199}N_{35}O_{44}S$	[2780-2789] [7)]		H	
523	685.5795	685.5873	4	$C_{114}H_{187}N_{33}O_{43}S$	[2781-2789] [7)]		H	
524	548.6636	548.6714	5				H	
525	861.4252	861.4325	4	$C_{150}H_{236}N_{42}O_{49}S_1$	[2790-2805]		X	K2804
526	689.3420	689.3470	5			X	X	
527	574.6190	574.6237	6			X	X	
528	718.8617	718.8663	4	$C_{126}H_{198}N_{36}O_{39}S_1$	[2790-2805] [5)]	X	X	

529	748.3428	748.3491	6	$C_{195}H_{294}N_{52}O_{64}S_3$	[2845-2867]	X	X	K2852
530	897.8124	897.8175	5			X	X	
531	901.0119	901.0165	5	$C_{195}H_{294}N_{52}O_{65}S_3$	[2845-2867] [8)]	X	X	
532	979.4478	979.4539	4	$C_{171}H_{256}N_{46}O_{54}S_3$	[2845-2867] [5)]	X	X	
533	783.7573	783.7651	5			X	X	
534	872.4211	872.4246	3	$C_{112}H_{179}N_{31}O_{37}S_2$	[2845-2857] [5)]	X	X	
535	797.1331	797.1365	4	$C_{136}H_{217}N_{37}O_{47}S_2$	[2845-2857]	X		
536	1027.4949	1027.4937	5	$C_{222}H_{346}N_{60}O_{74}S_3$	[2853-2882]	X	X	K2874
537	856.4172	856.4126	6			X	X	
538	734.2055	734.2123	7				X	
539	736.4999	736.4974	7	$C_{222}H_{346}N_{60}O_{75}S_3$	[2853-2882] [8)]		X	
540	913.4352	913.4412	5	$C_{198}H_{308}N_{54}O_{64}S_3$	[2853-2882] [5)]	X	X	
541	761.3627	761.3690	6			X	X	
542	799.6550	799.6605	4	$C_{136}H_{227}N_{37}O_{49}S_1$	[2868-2882]	X	X	
543	875.7863	875.7899	3	$C_{112}H_{189}N_{31}O_{39}S_1$	[2868-2882] [5)]	X	X	
544	661.5896	661.5975	4	$C_{112}H_{191}N_{31}O_{40}S_1$	[2868-2882] [5,7)]		H	
545	804.1558	804.1637	4	$C_{136}H_{229}N_{37}O_{50}S_1$	[2868-2882] [7)]		H	
546	643.5247	643.5325	5				H	
547	721.1510	721.1589	5	$C_{153}H_{249}N_{43}O_{53}S_2$	[2875-2893]		X	K2882
548	758.6255	758.6304	4	$C_{129}H_{211}N_{37}O_{43}S_2$	[2875-2893] [5)]	X	X	
549	810.3817	810.3806	4	$C_{135}H_{212}N_{42}O_{47}S_2$	[2883-2897]	X	X	K2893
550	534.4468	534.4535	5	$C_{111}H_{174}N_{36}O_{37}S_2$	[2883-2897] [5)]	X		
551	667.8070	667.8149	4			X		
552	496.4720	496.4776	4	$C_{81}H_{123}N_{29}O_{28}S_1$	[2888-2896] [5)]	X	X	
553	517.2222	517.2278	4	$C_{84}H_{124}N_{30}O_{30}S_1$	[2897-2904]	X		K2897
554	538.5373	538.5460	7	$C_{158}H_{243}N_{53}O_{53}S_1$	[2894-2910]		X	
555	674.3219	674.3275	5	$C_{140}H_{223}N_{45}O_{50}S_1$	[2910-2924]	X	X	K2910
556	562.1007	562.1080	6				X	
557	481.9446	481.9508	7				X	
558	700.0848	700.0919	4	$C_{116}H_{185}N_{39}O_{40}S_1$	[2910-2924] [5)]	X		
559	855.3878	855.3939	6	$C_{222}H_{328}N_{62}O_{75}S_2$	[2925-2955] [6)]	X	X	K2929
560	926.0916	926.0959	3	$C_{116}H_{182}N_{32}O_{45}S_1$	[2925-2934]	X		
561	1103.5052	1103.5077	2	$C_{92}H_{144}N_{26}O_{35}S_1$	[2925-2934] [5)]	X		
562	736.0046	736.0076	3			X		
563	994.0436	994.0474	5	$C_{211}H_{313}N_{61}O_{75}S_2$	[2930-2959] [6)]	X	X	K2955
564	828.5431	828.5405	6			X	X	
565	710.3166	710.3215	7			X	X	
566	733.4903	733.4969	6	$C_{187}H_{275}N_{55}O_{65}S_2$	[2930-2959] [6,5)]	X		
567	879.9897	879.9948	5			X	X	
568	1099.7371	1099.7415	4			X		
569	712.8871	712.8950	7	$C_{211}H_{315}N_{61}O_{76}S_2$	[2930-2959] [6,7)]		H	

570	930.443	930.4433	6	$C_{252}H_{362}N_{66}O_{77}S_1$	[2987-3021]	X	X	K2987
571	1116.3256	1116.3304	5			X	X	
572	1395.1649	1395.1613	4			X	X	
573	912.7641	912.7693	3	$C_{118}H_{182}N_{32}O_{41}S_1$	[3038-3047]	X	X	K3044
574	684.8226	684.8293	4			X		
575	1083.5169	1083.5178	2	$C_{94}H_{144}N_{26}O_{31}S_1$	[3038-3047] [5)]	X	X	
576	722.6833	722.6815	3				X	
577	841.0538	841.0609	3	$C_{109}H_{165}N_{29}O_{38}S_1$	[3038-3047] [9)]	X		
578	842.7167	842.7211	3	$C_{105}H_{168}N_{28}O_{40}S_2$	[3087-3094]	X	X	K3087
579	848.0482	848.0533	3	$C_{105}H_{168}N_{28}O_{41}S_2$	[3087-3094] [8)]	X	X	
580	978.4405	978.4455	2	$C_{81}H_{130}N_{22}O_{30}S_2$	[3087-3094] [5)]	X	X	
581	652.6338	652.6333	3				X	
582	986.4429	986.4435	2	$C_{81}H_{130}N_{22}O_{31}S_2$	[3087-3094] [5,8)]		X	
583	657.9644	657.9650	3				X	
584	935.1105	935.1184	3	$C_{119}H_{191}N_{33}O_{41}S_2$	[3078-3094] [5)]		X	
585	940.4458	940.4500	3	$C_{119}H_{191}N_{33}O_{42}S_2$	[3078-3094] [5,8)]	X	X	
586	848.1564	848.1557	4	$C_{143}H_{229}N_{39}O_{52}S_2$	[3078-3094] [8)]		X	
587	844.1477	844.1564	4	$C_{143}H_{229}N_{39}O_{51}S_2$	[3078-3094]	X	X	
588	1027.5074	1027.5261	3	$C_{137}H_{214}N_{38}O_{41}S_1$	[3112-3122]		X	K3121
589	770.8859	770.8965	4				X	
590	837.4347	837.4373	3	$C_{113}H_{176}N_{32}O_{31}S_1$	[3112-3122] [5)]	X		
591	528.7609	528.7686	4	$C_{87}H_{146}N_{28}O_{31}S_1$	[3119-3122]		X	
592	772.1672	772.1728	5	$C_{168}H_{254}N_{48}O_{55}S_1$	[3170-3192] [5)]	X		K3173
593	1107.5271	1107.5309	4	$C_{192}H_{292}N_{54}O_{65}S_1$	[3170-3192]		X	
594	886.2199	886.2258	5			X	X	
595	738.6832	738.6893	6			X	X	
596	780.1026	780.1085	4	$C_{135}H_{197}N_{39}O_{45}S_1$	[3170-3186] [5)]	X		
597	775.7676	775.7755	5	$C_{168}H_{256}N_{48}O_{56}S_1$	[3170-3192] [5,7)]		H	
598	741.6838	741.6917	6	$C_{192}H_{294}N_{54}O_{66}S_1$	[3170-3192] [7)]		H	
599	691.0121	691.0128	3	$C_{85}H_{143}N_{27}O_{31}S_1$	[3170-3192]		X	K3197
600	518.5114	518.5114	4				X	
601	418.6054	418.6132	5	$C_{85}H_{145}N_{27}O_{32}S_1$	[3196-3199] [7)]		H	
602	897.1288	897.1337	3	$C_{117}H_{193}N_{31}O_{39}S_1$	[3211-3220]	X	X	K3216
603	673.0966	673.1021	4			X	X	
604	707.0405	707.0454	3	$C_{93}H_{155}N_{25}O_{29}S_1$	[3211-3220] [5)]	X	X	
605	713.0416	713.0494	3	$C_{93}H_{155}N_{25}O_{29}S_1$	[3211-3220] [5,7)]		H	
606	677.5974	677.6053	4	$C_{117}H_{193}N_{31}O_{39}S_1$	[3211-3220] [7)]		H	
607	542.2779	542.2858	5				H	
608	1155.5181	1155.5214	4	$C_{198}H_{296}N_{52}O_{72}S_2$	[3221-3248]		X	K3240
609	953.9506	953.9567	4	$C_{169}H_{254}N_{44}O_{53}S_2$	[3229-3248]	X		
610	957.9491	957.9554	4	$C_{169}H_{254}N_{44}O_{54}S_2$	[3229-3248] [8)]	X		

611	770.3733	770.3792	3	$C_{101}H_{157}N_{27}O_{33}S_1$	[3229-3241] [5)]	X	X	
612	1155.0667	1155.0652	2			X		
613	841.0892	841.0883	3	$C_{110}H_{173}N_{31}O_{35}S_1$	[3270-3276]	X	X	K3275
614	631.068	631.0681	4			X	X	
615	505.0491	505.0565	5				X	
616	650.9940	651.0005	3	$C_{86}H_{135}N_{25}O_{25}S_1$	[3270-3276] [5)]	X	X	
617	488.4945	488.5024	4				X	
618	555.2761	555.2757	4	$C_{95}H_{152}N_{26}O_{33}S_1$	[3272-3276]	X	X	
619	549.9365	549.9440	3	$C_{71}H_{114}N_{20}O_{23}S_1$	[3272-3276] [5)]	X	X	
620	635.5634	635.5712	4	$C_{110}H_{175}N_{31}O_{36}S_1$	[3270-3276] [7)]		H	
621	508.6507	508.6586	5				H	
622	783.9791	783.9850	7	$C_{243}H_{390}N_{66}O_{76}S_1$	[3276-3310]		X	K3276
623	914.488	914.4807	6			X	X	
624	1097.1795	1097.1753	5			X	X	
625	819.4311	819.4370	6	$C_{219}H_{352}N_{60}O_{66}S_1$	[3276-3310] [5)]	X	X	
626	1228.6438	1228.6516	4				X	
627	926.9636	926.9707	4	$C_{161}H_{258}N_{44}O_{54}S_1$	[3276-3294]		X	
628	741.7731	741.7776	5			X	X	
629	917.4802	917.4830	6	$C_{243}H_{392}N_{66}O_{77}S_1$	[3276-3310] [7)]		H	
630	786.5534	786.5579	7				H	
631	781.5326	781.5407	8	$C_{278}H_{447}N_{75}O_{86}S_1$	[3276-3317]		X	K3310
632	893.0420	893.0454	7			X		
633	826.2252	826.2304	5	$C_{181}H_{292}N_{50}O_{58}S_1$	[3295-3317]	X	X	
634	1032.5346	1032.5363	4			X	X	
635	889.9662	889.9700	4	$C_{157}H_{254}N_{44}O_{48}S_1$	[3295-3317] [5)]		X	
636	1020.3621	1020.3692	6	$C_{272}H_{435}N_{73}O_{85}S_1$	[3277-3317]		X	
637	874.7403	874.7456	7			X	X	
638	829.8252	829.8331	5	$C_{181}H_{294}N_{50}O_{59}S_1$	[3295-3317]		X	
639	694.6140	694.6141	4	$C_{120}H_{199}N_{33}O_{40}S_1$	[3311-3321]	X	X	K3317
640	962.2581	962.2645	5	$C_{207}H_{332}N_{54}O_{67}S_5$	[3322-3350]		X	K3325
641	968.6546	968.6625	5	$C_{207}H_{332}N_{54}O_{69}S_5$	[3322-3350] [8)]		X	
642	965.4556	965.4635	5	$C_{207}H_{332}N_{54}O_{68}S_5$	[3322-3350] [8)]		X	
643	968.6537	968.6625	5	$C_{207}H_{332}N_{54}O_{69}S_5$	[3322-3350] [8)]	X	X	
644	942.4276	942.4312	3	$C_{118}H_{189}N_{31}O_{43}S_3$	[3323-3333]	X	X	
645	969.0578	969.0656	5	$C_{207}H_{334}N_{54}O_{69}S_5$	[3322-3350] [7,8)]		H	
646	1164.0449	1164.0432	4	$C_{200}H_{318}N_{50}O_{65}S_6$	[3326-3352] [6)]	X	X	K3350
647	1168.0371	1168.0425	4	$C_{200}H_{318}N_{50}O_{66}S_6$	[3326-3352] [6,8)]	X		
648	833.6492	833.6523	4	$C_{148}H_{223}N_{39}O_{45}S_2$	[3351-3365] [6)]	X	X	K3352
649	667.1186	667.1233	5			X	X	
650	691.0803	691.0866	4	$C_{124}H_{185}N_{33}O_{35}S_2$	[3351-3365] [6, 5)]	X	X	
651	1148.6885	1148.6906	6	$C_{299}H_{445}N_{79}O_{101}S_4$	[3353-3398]	X	X	K3365

652	984.739	984.7358	7			X	X	
653	1192.5357	1192.5397	5	$C_{258}H_{385}N_{67}O_{88}S_4$	[3353-3390] [8]	X		
654	832.0572	832.0583	3	$C_{105}H_{168}N_{28}O_{38}S_2$	[3363-3370]	X	X	
655	837.3845	837.3900	3	$C_{105}H_{168}N_{28}O_{39}S_2$	[3363-3370] [8]	X	X	
656	962.4481	962.4506	2	$C_{81}H_{130}N_{22}O_{28}S_2$	[3363-3370] [5]	X	X	
657	641.9653	641.9700	3			X	X	

[1] Numbers inside brackets correspond to the position of the proteolytic peptide within the sequence of KLH2. All peptides from KLH2 shown in this table are linked to (C^1-K^{16}) fragment of Cys^1pP0, except those peptides where it is specified if they are linked to (C^1-K^{11}), (C^1-K^{14}) or (C^1-K^{17}) fragment of Cys^1pP0.
[2] Identification of type 2 peptides in the KLH2-Cys^1pP0 conjugate using pLink2 software [2].
[3] Identification of type 2 peptides in the KLH2-Cys^1pP0 conjugate using Kojak software [3].
[4] Indicates the position where the peptide Cys^1pP0 is added by the Michael addition to the free amino groups in the Lys residues or *N*-terminus of the KLH2.
[5] Peptide from KLH1 linked to (C^1-K^{11}) fragment of Cys^1pP0
[6] Carbamidomethylation of Cys
[7] Identification of type 2 peptides with the hydrolyzed linker
[8] Met→ Met sulfoxide
[9] Peptide from KLH1 linked to (C^1-K^{14}) fragment of Cys^1pP0

Table S7. Identification of conjugation sites in KLH2-Cys[1]pP0 conjugate using Kojak [2] and pLink2 [3] software. Type 2 peptides were identified using transcyclized and hydrolyzer linker.

#	*m/z* exp.	*m/z* theor.	*z*	Elemental composition	Assignment [1)]	pLink [2)]	Kojak [3)]	Conjugation site [4)]
1	907.4576	907.4655	2	$C_{75}H_{128}N_{24}O_{26}S$	[1-7] [5)]		X	Nt
2	605.3050	605.3129	3				X	
3	795.3933	795.4012	3	$C_{99}H_{166}N_{30}O_{36}S$	[1-7]		X	
4	596.7950	596.8029	4				X	
5	477.6360	477.6439	5				X	
6	601.2979	601.3055	4	$C_{99}H_{168}N_{30}O_{37}S$	[1-7] [6)]		H	
7	503.2550	503.2628	5	$C_{105}H_{178}N_{32}O_{37}S$	[1-7] [7)]		X	
8	854.1786	854.1860	4	$C_{143}H_{241}N_{41}O_{53}S$	[1-22] [5)]		X	K7
9	996.7448	996.7527	4	$C_{167}H_{279}N_{47}O_{63}S$	[1-22]		X	
10	797.5958	797.6037	5				X	
11	801.1958	801.2058	5	$C_{167}H_{281}N_{47}O_{64}S$	[1-22] [6)]		H	
12	1045.9611	1045.9690	2	$C_{83}H_{135}N_{25}O_{36}S$	[7-17] [5)]		X	
13	887.7290	887.7369	3	$C_{107}H_{173}N_{31}O_{46}S$	[7-17]		X	
14	915.44443	915.4523	3	$C_{114}H_{190}N_{32}O_{44}S$	[7-22] [5)]	X	X	
15	829.4017	829.4074	4	$C_{138}H_{228}N_{38}O_{54}S$	[7-22]	X	X	
16	1477.4248	1477.4322	4	$C_{247}H_{389}N_{69}O_{93}S_3$	[8-52] [5,8)]		X	K22
17	1176.0241	1176.0320	4	$C_{196}H_{302}N_{58}O_{71}S_3$	[23-55] [5,8)]		X	K52
18	941.01926	941.0272	5				X	
19	944.2197	944.2261	5	$C_{196}H_{302}N_{58}O_{72}S_3$	[23-55] [5,8,9)]	X		
20	1318.5976	1318.5983	4	$C_{220}H_{340}N_{64}O_{81}S_3$	[23-55] [8)]	X	X	
21	1055.0799	1055.0801	5			X	X	
22	879.4011	879.4014	6			X	X	
23	756.4802	756.4896	7	$C_{220}H_{342}N_{64}O_{82}S_3$	[23-55] [8,6)]		H	
24	1058.2797	1058.2792	5	$C_{220}H_{340}N_{64}O_{82}S_3$	[23-55] [8,9)]	X	X	
25	882.0594	882.0673	6			X	X	
26	763.3396	763.3475	3	$C_{96}H_{142}N_{32}O_{32}S$	[117-127] [5)]		X	K119
27	572.7547	572.7625	4			X	X	
28	715.32192	715.3288	4	$C_{120}H_{180}N_{38}O_{42}S$	[117-127]	X		
29	572.45842	572.4646	5			X		
30	1026.1641	1026.1619	3	$C_{134}H_{202}N_{40}O_{42}S_1$	[120-136] [5)]	X	X	K135
31	769.8740	769.8734	4			X	X	
32	616.1002	616.1002	5			X	X	
33	1216.2505	1216.2501	3	$C_{158}H_{240}N_{46}O_{52}S_1$	[120-136]	X	X	
34	912.4400	912.4396	4			X	X	
35	730.1538	730.1533	5			X	X	
36	608.6288	608.6290	6			X	X	
37	619.6924	619.7023	5	$C_{134}H_{204}N_{40}O_{43}S_1$	[120-136] [5,6)]		H	
38	916.9351	916.9422	4	$C_{158}H_{242}N_{46}O_{53}S_1$	[120-136] [6)]		H	
39	733.7454	733.7554	5				H	
40	611.6211	611.6307	6				H	
41	1024.0102	1024.0181	2	$C_{88}H_{143}N_{25}O_{29}S_1$	[128-136] [5)]	X		
42	683.0157	683.0146	3			X		
43	873.1030	873.1030	3	$C_{112}H_{181}N_{31}O_{39}S_1$	[128-136]	X		

44	655.0790	655.0792	4			X	X	
45	515.4950	515.5028	4	$C_{83}H_{139}N_{27}O_{32}S$	[136-139]		X	**K136**
46	641.3182	641.3242	4	$C_{107}H_{176}N_{34}O_{37}S$	[136-148] [5)]	X		
47	513.2546	513.2609	5			X		
48	627.3134	627.3140	5	$C_{131}H_{214}N_{40}O_{47}S_1$	[136-148]	X	X	
49	522.9293	522.9296	6			X	X	
50	873.9180	873.9258	6	$C_{222}H_{353}N_{67}O_{74}S_3$	[137-172] [5,8)]	X		**K148**
51	876.5838	876.5917	6	$C_{222}H_{353}N_{67}O_{75}S_3$	[137-172] [5,8,9)]		X	
52	968.9621	968.9700	6	$C_{246}H_{391}N_{73}O_{84}S_3$	[137-172] [8)]		X	
53	832.9668	832.9747	7	$C_{246}H_{391}N_{73}O_{85}S_3$	[137-172] [8,9)]	X	X	
54	596.2871	596.2949	6	$C_{151}H_{238}N_{48}O_{51}S_1$	[140-156]		X	
55	612.3069	612.3071	4	$C_{105}H_{164}N_{34}O_{32}S_1$	[145-156] [5)]	X	X	
56	490.0476	490.0473	5			X	X	
57	754.8726	754.8734	4	$C_{129}H_{202}N_{40}O_{42}S_1$	[145-156]	X	X	
58	604.0999	604.1002	5			X	X	
59	503.5841	503.5848	6			X	X	
60	526.2548	526.2612	5	$C_{109}H_{175}N_{37}O_{37}S$	[148-156]	X		
61	876.9180	876.9276	6	$C_{222}H_{355}N_{67}O_{75}S_3$	[137-172] [6,5)]		H	
62	971.9621	971.9717	6	$C_{246}H_{393}N_{73}O_{85}S_3$	[137-172] [6)]		H	
63	616.8019	616.8098	4	$C_{105}H_{166}N_{34}O_{33}S_1$	[145-156] [6,5)]		H	
64	493.6415	493.6494	5				H	
65	759.3677	759.3760	4	$C_{129}H_{204}N_{40}O_{43}S_1$	[145-156] [6)]		H	
66	607.6924	607.7023	5				H	
67	506.5770	506.5866	6				H	
68	905.6509	905.6588	4	$C_{150}H_{231}N_{47}O_{52}S_3$	[230-252] [5,8)]		X	**K231**
69	724.7207	724.7286	5			X	X	
70	727.9207	727.9276	5	$C_{150}H_{231}N_{47}O_{53}S_3$	[230-252] [5,8,9)]	X		
71	838.7754	838.7816	5	$C_{174}H_{269}N_{53}O_{62}S_3$	[230-252] [8)]	X	X	
72	701.8110	701.8184	6	$C_{174}H_{269}N_{53}O_{63}S_3$	[230-252] [8,9)]	X	X	
73	775.0266	775.0275	6	$C_{193}H_{302}N_{60}O_{68}S_3$	[230-261] [5,8)]	X	X	
74	870.0695	870.0717	6	$C_{217}H_{340}N_{66}O_{78}S_3$	[230-261] [8)]	X	X	
75	872.7302	872.7375	6	$C_{217}H_{340}N_{66}O_{79}S_3$	[230-261] [8,9)]	X		
76	623.2757	623.2836	4	$C_{105}H_{156}N_{32}O_{37}S$	[262-274] [5)]		X	**K265**
77	765.8486	765.8490	4	$C_{129}H_{194}N_{38}O_{47}S_1$	[262-274]	X	X	
78	612.8839	612.8814	5			X	X	
79	627.7788	627.7862	4	$C_{105}H_{158}N_{32}O_{38}S$	[262-274] [5,6)]		H	
80	502.4230	502.4305	5				H	
81	770.3451	770.3525	4	$C_{129}H_{196}N_{38}O_{48}S_1$	[262-274] [6)]		H	
82	616.4761	616.4835	5				H	
83	513.8967	513.9042	6				H	
84	524.5907	524.5919	3	$C_{63}H_{106}N_{22}O_{23}S_1$	[300-304] [5)]		X	**K302**
85	720.6757	720.6837	3	$C_{87}H_{146}N_{28}O_{34}S$	[300-304] [6)]		H	
86	540.7568	540.7648	4				H	
87	432.8054	432.8134	5				H	
88	1063.8282	1063.8361	3	$C_{145}H_{209}N_{37}O_{41}S_2$	[340-358] [5)]		X	
89	798.1291	798.1290	4			X	X	
90	1253.9211	1253.9244	3	$C_{169}H_{247}N_{43}O_{51}S_2$	[340-358]	X	X	

91	940.6943	940.6953	4			X	X	**K353**
92	752.7499	752.7578	5				X	
93	944.6950	944.6953	4	$C_{169}H_{247}N_{43}O_{52}S_2$	[340-358] [9]	X	X	
94	981.1113	981.1191	6	$C_{266}H_{374}N_{68}O_{81}S_2$	[340-382] [5]	X	X	
95	841.0954	841.1032	7				X	
96	1076.1554	1076.1633	6	$C_{290}H_{412}N_{74}O_{91}S_2$	[340-382]	X	X	
97	922.5618	922.5696	7			X	X	
98	807.3666	807.3745	8				X	
99	1078.8212	1078.8291	6	$C_{290}H_{412}N_{74}O_{92}S_2$	[340-382] [9]		X	
100	924.8478	924.8546	7			X	X	
101	809.3659	809.3738	8				X	
102	662.3027	662.3106	3	$C_{88}H_{129}N_{25}O_{24}S_2$	[352-358] [5]	X	X	
103	667.6369	667.6423	3	$C_{88}H_{129}N_{25}O_{25}S_2$	[352-358] [5,9]	X	X	
104	643.5420	643.5499	4	$C_{112}H_{167}N_{31}O_{35}S_2$	[352-358] [9]	X	X	
105	945.1905	945.1979	4	$C_{169}H_{249}N_{43}O_{52}S_2$	[340-358] [6]		H	
106	756.3524	756.3599	5				H	
107	759.5511	759.5589	5	$C_{169}H_{249}N_{43}O_{53}S_2$	[340-358] [6,9]		H	
108	984.1128	984.1209	6	$C_{266}H_{376}N_{68}O_{82}S_2$	[340-382] [5,6]		H	
109	756.7852	756.7921	5	$C_{165}H_{263}N_{49}O_{51}S$	[407-427]	X		**K409**
110	659.6284	659.6354	7	$C_{202}H_{324}N_{62}O_{60}S_1$	[400-427]		X	**K414**
111	729.1179	729.1257	4	$C_{127}H_{201}N_{39}O_{38}S$	[410-427] [5]		X	
112	871.6841	871.6920	4	$C_{151}H_{239}N_{45}O_{48}S$	[410-427]		X	
113	697.5500	697.5551	5			X	X	
114	1014.5306	1014.5300	3	$C_{133}H_{213}N_{41}O_{39}S_1$	[410-428] [5]		X	
115	761.1416	761.1495	4				X	
116	609.1210	609.1212	5			X	X	
117	1204.6104	1204.6183	3	$C_{157}H_{251}N_{47}O_{49}S_1$	[410-428]		X	
118	903.7161	903.7157	4			X	X	
119	723.1746	723.1741	5			X	X	
120	602.8055	602.8130	6			X	X	
121	516.8330	516.8409	7				X	
122	765.6441	765.6521	4	$C_{133}H_{215}N_{41}O_{40}S_1$	[410-428] [5,6]		H	
123	510.7628	510.7707	6				H	
124	908.2117	908.2183	4	$C_{157}H_{253}N_{47}O_{50}S_1$	[410-428] [6]		H	
125	726.7694	726.7762	5				H	
126	605.8078	605.8148	6				H	
127	519.4067	519.4138	7				H	
128	922.1135	922.1123	3	$C_{115}H_{186}N_{34}O_{43}S_1$	[428-442] [5]	X	X	**K428**
129	834.3945	834.4024	4	$C_{139}H_{224}N_{40}O_{53}S$	[428-442]		X	
130	1114.2825	1114.2806	4	$C_{186}H_{297}N_{55}O_{68}S_2$	[429-452]	X	X	**K443**
131	743.1893	743.1898	6			X		
132	551.2623	551.2629	4	$C_{89}H_{148}N_{28}O_{33}S_2$	[443-447]		X	
133	555.7566	555.7656	4	$C_{89}H_{150}N_{28}O_{34}S_2$	[443-447] [6]		H	
134	444.8053	444.8140	5				H	
135	555.2615	555.2617	4	$C_{89}H_{148}N_{28}O_{34}S_2$	[443-447] [9]		X	
136	961.2509	961.2588	5	$C_{204}H_{317}N_{63}O_{66}S_3$	[444-476] [5,8]	X	X	
137	801.2091	801.2170	6			X	X	

138	1075.3039	1075.3118	5	$C_{228}H_{355}N_{69}O_{76}S_3$	[444-476] [8)]		X	**K452**
139	896.2532	896.2611	6				X	
140	768.3610	768.3678	7			X	X	
141	898.9203	898.9269	6	$C_{228}H_{355}N_{69}O_{77}S_3$	[444-476] [8,9)]	X	X	
142	770.6460	770.6528	7			X	X	
143	674.4393	674.4471	8				X	
144	873.4177	873.4171	4	$C_{151}H_{228}N_{44}O_{50}S_1$	[448-469] [5)]	X	X	
145	1015.9854	1015.9833	4	$C_{175}H_{266}N_{50}O_{60}S_1$	[448-469]	X	X	
146	812.9876	812.9882	5			X	X	
147	899.2565	899.2629	6	$C_{228}H_{357}N_{69}O_{77}S_3$	[444-476] [6,8)]		H	
148	674.6924	674.6991	8				H	
149	877.9097	877.9197	4	$C_{151}H_{230}N_{44}O_{51}S_1$	[448-469] [5,6)]		H	
150	702.5277	702.5374	5				H	
151	816.5836	816.5903	5	$C_{175}H_{268}N_{50}O_{61}S_1$	[448-469] [6)]		H	
152	704.6609	704.6624	3	$C_{84}H_{138}N_{30}O_{30}S_2$	[470-478] [5,8)]	X	X	**K476**
153	528.7483	528.7487	4			X	X	
154	671.3071	671.3150	4	$C_{108}H_{176}N_{36}O_{40}S_2$	[470-478] [8)]	X	X	
155	537.2457	537.2535	5			X	X	
156	766.8545	766.8624	6	$C_{203}H_{299}N_{55}O_{64}S_2$	[615-639]		X	**K615**
157	659.7317	659.7396	7	$C_{203}H_{299}N_{55}O_{65}S_2$	[615-639] [9)]		X	
158	542.7535	542.7632	4	$C_{90}H_{146}N_{26}O_{34}S$	[652-656] [6)]		H	**K653**
159	906.0205	906.0284	5	$C_{191}H_{297}N_{57}O_{67}S_2$	[657-682] [8)]		X	**K669**
160	755.1837	755.1916	6				X	
161	948.6313	948.6281	5	$C_{200}H_{304}N_{56}O_{72}S_3$	[703-728]	X	X	**K722**
162	790.6922	790.6913	6			X	X	
163	780.0687	780.0674	3	$C_{103}H_{164}N_{28}O_{32}S_1$	[756-768] [5)]	X	X	**K757**
164	727.8685	727.8687	4	$C_{127}H_{202}N_{34}O_{42}S_1$	[756-768]	X	X	
165	812.3994	812.4073	3	$C_{104}H_{171}N_{29}O_{34}S_2$	[758-771] [5)]		X	**K768**
166	1002.4937	1002.4956	3	$C_{128}H_{209}N_{35}O_{44}S_2$	[758-771]	X	X	
167	752.1241	752.1237	4			X	X	
168	756.1213	756.1224	4	$C_{128}H_{209}N_{35}O_{45}S_2$	[758-771] [9)]	X	X	
169	605.4955	605.5026	5	$C_{128}H_{211}N_{35}O_{45}S_2$	[758-771] [6)]		H	
170	630.7776	630.7836	4	$C_{108}H_{162}N_{30}O_{34}S_3$	[769-779] [5,9)]	X		**K771**
171	612.4893	612.4835	5	$C_{132}H_{200}N_{36}O_{42}S_3$	[769-779]		X	
172	773.3420	773.3499	4	$C_{132}H_{200}N_{36}O_{44}S_3$	[769-779] [9)]		X	
173	618.8736	618.8815	5				X	
174	525.98605	525.9939	4	$C_{86}H_{133}N_{29}O_{31}S$	[826-835] [5)]		X	**K829**
175	939.9375	939.9352	4	$C_{163}H_{242}N_{46}O_{53}S_2$	[864-888] [5,8)]	X	X	**K879**
176	1082.4936	1082.5015	4	$C_{187}H_{280}N_{52}O_{63}S_2$	[864-888] [8)]		X	
177	866.2018	866.2028	5			X		
178	743.6663	743.6742	3	$C_{94}H_{145}N_{27}O_{32}S_2$	[880-889] [5,8)]	X	X	**K888**
179	700.5660	700.5738	4	$C_{118}H_{183}N_{33}O_{42}S_2$	[880-889] [8)]	X	X	
180	940.10267	940.1105	3	$C_{127}H_{180}N_{36}O_{36}S_1$	[917-931] [5)]		X	**K917**
181	705.3340	705.3348	4			X	X	
182	847.9018	847.9011	4	$C_{151}H_{218}N_{42}O_{46}S_1$	[917-931]	X	X	
183	678.5237	678.5225	5			X	X	
184	568.0633	568.0716	5	$C_{127}H_{182}N_{36}O_{37}S_1$	[917-931] [5,6)]		H	

185	852.3962	852.4037	4	$C_{151}H_{220}N_{42}O_{47}S_1$	[917-931] [6]		H	
186	682.1170	682.1246	5				H	
187	568.5975	568.6051	6				H	
188	633.1155	633.1231	5	$C_{141}H_{217}N_{39}O_{42}S$	[1051-1062] [6]		H	**K1060**
189	806.1214	806.1253	4	$C_{132}H_{213}N_{41}O_{47}S_3$	[1063-1077] [8]	X	X	**K1064**
190	810.6210	810.6279	4	$C_{132}H_{215}N_{41}O_{48}S_3$	[1063-1077] [6]		H	
191	648.6968	648.7039	5				H	
192	871.2720	871.2799	7	$C_{266}H_{407}N_{75}O_{84}S_3$	[1065-1108] [5,8]		X	**K1078**
193	1111.3615	1111.3694	6	$C_{290}H_{445}N_{81}O_{94}S_3$	[1065-1108] [8]		X	
194	952.7395	952.7463	7			X	X	
195	1046.8442	1046.8441	3	$C_{134}H_{212}N_{38}O_{47}S_1$	[1078-1096] [5]	X	X	
196	1236.9245	1236.9324	3	$C_{158}H_{250}N_{44}O_{57}S_1$	[1078-1096]		X	
197	927.9522	927.9512	4			X	X	
198	742.5630	742.5626	5			X		
199	798.9866	798.9944	5	$C_{173}H_{268}N_{50}O_{57}S$	[1078-1103] [5]	X	X	
200	913.0473	913.0474	5	$C_{197}H_{306}N_{56}O_{67}S_1$	[1078-1103]	X	X	
201	761.0397	761.0408	6			X	X	
202	789.8799	789.8876	4	$C_{134}H_{214}N_{38}O_{48}S_1$	[1078-1096] [5,6]		H	
203	932.4474	932.4539	4	$C_{158}H_{252}N_{44}O_{58}S_1$	[1078-1096] [6]		H	
204	746.1579	746.1647	5				H	
205	668.9888	668.9884	6	$C_{173}H_{270}N_{50}O_{58}S$	[1078-1103] [5,6]		H	
206	655.0302	655.0376	7	$C_{197}H_{308}N_{56}O_{68}S_1$	[1078-1103] [6]		H	
207	1600.4044	1600.4122	3	$C_{212}H_{312}N_{54}O_{72}S$	[1104-1130]		X	**K1108**
208	960.6426	960.6505	5				X	
209	1062.4886	1062.4976	4	$C_{188}H_{276}N_{48}O_{63}S$	[1104-1130] [5,6]		H	
210	918.65258	918.6605	5	$C_{204}H_{314}N_{56}O_{61}S_2$	[1137-1162] [8]		X	**K1157**
211	837.4176	837.4231	3	$C_{110}H_{176}N_{30}O_{33}S_2$	[1150-1162] [5,8]	X	X	
212	955.7945	955.8024	3	$C_{125}H_{197}N_{33}O_{40}S_2$	[1150-1162] [8,10]	X	X	
213	770.8816	770.8855	4	$C_{134}H_{214}N_{36}O_{43}S_2$	[1150-1162] [8]	X	X	
214	616.9021	616.9100	5				X	
215	922.2545	922.2626	5	$C_{204}H_{316}N_{56}O_{62}S_2$	[1137-1162] [6,8]		H	
216	768.7121	768.7201	6				H	
217	757.0129	757.0201	3	$C_{98}H_{149}N_{25}O_{35}S$	[1191-1195]		X	**K1193**
218	63.1072	763.1150	4	$C_{135}H_{201}N_{35}O_{44}S$	[1205-1216]	X	X	**K1214**
219	979.4557	979.4598	2	$C_{88}H_{128}N_{22}O_{27}S$	[1210-1216] [5]	X	X	
220	653.3034	653.3091	3			X	X	
221	843.3900	843.3975	3	$C_{112}H_{166}N_{28}O_{37}S$	[1210-1216]	X	X	
222	913.0583	913.0662	5	$C_{196}H_{318}N_{56}O_{67}S$	[1262-1292] [5]		X	**K1283**
223	1283.6479	1283.6470	4	$C_{220}H_{356}N_{62}O_{77}S_1$	[1262-1292]		X	
224	1027.1216	1027.1191	5			X	X	
225	856.1015	856.1006	6			X	X	
226	1031.0041	1031.0077	2	$C_{88}H_{141}N_{25}O_{30}S$	[1276-1284] [5]	X	X	
227	687.6691	687.6744	3			X	X	
228	877.7574	877.7627	3	$C_{112}H_{179}N_{31}O_{40}S$	[1276-1284]	X	X	
229	658.5661	658.574	4				X	
230	983.8323	983.8312	3	$C_{129}H_{205}N_{35}O_{42}S_1$	[1276-1292] [5]	X	X	
231	1173.9116	1173.9196	3	$C_{153}H_{243}N_{41}O_{52}S_1$	[1276-1292]		X	

232	880.6933	880.6916	4			X	X	
233	916.6610	916.6683	5	$C_{196}H_{320}N_{56}O_{68}S$	[1276-1292] [6,5)]		H	
234	764.0508	764.0582	6				H	
235	885.1874	885.1943	4	$C_{153}H_{245}N_{41}O_{53}S_1$	[1276-1292] [6)]		H	
236	835.0730	835.0732	3	$C_{109}H_{167}N_{31}O_{35}S_1$	[1284-1296] [5)]	X	X	**K1292**
237	626.5574	626.5569	4			X	X	
238	1025.1645	1025.1615	3	$C_{133}H_{205}N_{37}O_{45}S_1$	[1284-1296]	X	X	
239	769.1233	769.1231	4			X	X	
240	615.5006	615.5006	5			X	X	
241	637.9826	637.9885	3	$C_{82}H_{130}N_{26}O_{25}S$	[1289-1296] [5)]	X	X	
242	478.7372	478.7433	4			X	X	
243	621.3017	621.3096	4	$C_{106}H_{168}N_{32}O_{35}S$	[1289-1296]		X	
244	773.6181	773.6257	4	$C_{133}H_{207}N_{37}O_{46}S_1$	[1284-1296] [6)]		H	
245	619.0945	619.1022	5				H	
246	516.0788	516.0864	6				H	
247	681.3048	681.3127	3	$C_{86}H_{132}N_{26}O_{28}S_2$	[1293-1301] [5,8)]		X	**K1296**
248	653.7967	653.8027	4	$C_{110}H_{170}N_{32}O_{38}S_2$	[1293-1301] [8)]	X		
249	1261.0921	1261.0956	4	$C_{222}H_{330}N_{58}O_{75}S_1$	[1336-1366]	X	X	**1349**
250	1009.0786	1009.0781	5			X	X	
251	914.1036	914.1085	3	$C_{114}H_{186}N_{32}O_{44}S$	[1349-1359]	X	X	
252	1003.8099	1003.8177	3	$C_{128}H_{201}N_{37}O_{45}S$	[1349-1366] [5)]		X	
253	895.6736	895.6815	4	$C_{152}H_{239}N_{43}O_{55}S$	[1349-1366]		X	
254	1123.0256	1123.0320	4	$C_{198}H_{294}N_{52}O_{66}S$	[1336-1366] [5,6)]		H	
255	933.0779	933.0858	3	$C_{122}H_{177}N_{31}O_{43}S$	[1395-1403]		X	**K1399**
256	1003.4851	1003.4843	4	$C_{180}H_{264}N_{48}O_{55}S_1$	[1436-1461] [5)]	X	X	**K1437**
257	917.0454	917.0419	5	$C_{204}H_{302}N_{54}O_{65}S_1$	[1436-1461]	X	X	
258	655.3101	655.3179	7				X	
259	806.5812	806.5911	5	$C_{180}H_{266}N_{48}O_{56}S_1$	[1436-1461] [5,6)]		H	
260	672.3176	672.3272	6				H	
261	767.3617	767.3713	6	$C_{204}H_{304}N_{54}O_{66}S_1$	[1436-1461] [6)]		H	
262	657.8815	657.8909	7				H	
263	739.9977	740.0081	3	$C_{93}H_{144}N_{26}O_{35}S$	[1475-1479]		X	**K1475**
264	706.3223	706.3224	4	$C_{115}H_{184}N_{36}O_{41}S_3$	[1475-1489] [5,8)]	X	X	
265	848.8807	848.8886	4	$C_{139}H_{222}N_{42}O_{51}S_3$	[1475-1489] [8)]		X	
266	679.3126	679.3124	5			X	X	
267	682.5050	682.5114	5	$C_{139}H_{222}N_{42}O_{52}S_3$	[1475-1489] [8,9)]	X	X	
268	906.5835	906.5913	6	$C_{228}H_{361}N_{65}O_{81}S_4$	[1475-1507] [8,9)]		X	
269	682.9053	682.9146	5	$C_{139}H_{224}N_{42}O_{52}S_3$	[1475-1489] [8,6)]		H	
270	970.4482	970.4561	5	$C_{204}H_{323}N_{59}O_{70}S_4$	[1475-1507] [5,8)]	X	X	**K1489**
271	1084.5012	1084.5090	5	$C_{228}H_{361}N_{65}O_{80}S_4$	[1475-1507] [8)]	X	X	
272	903.92113	903.9255	6			X	X	
273	1087.7001	1087.7080	5	$C_{228}H_{361}N_{65}O_{81}S_4$	[1475-1507] [8,9)]		X	
274	906.5835	906.5913	6				X	
275	1180.7865	1180.7944	4	$C_{198}H_{311}N_{57}O_{69}S_4$	[1476-1507] [5,8)]	X	X	
276	1058.8836	1058.8900	5	$C_{222}H_{349}N_{63}O_{79}S_4$	[1476-1507] [8)]	X	X	
277	1062.0812	1062.0890	5	$C_{222}H_{349}N_{63}O_{80}S_4$	[1476-1507] [8,9)]		X	
278	917.7656	917.7735	3	$C_{118}H_{183}N_{33}O_{41}S$	[1489-1498]	X	X	

279	1057.5153	1057.5135	3	$C_{135}H_{216}N_{38}O_{46}S_2$	[1489-1507] [5)]		X	
280	1062.8396	1062.8452	3	$C_{135}H_{216}N_{38}O_{47}S_2$	[1489-1507] [5,9)]	X		
281	935.9540	935.9534	4	$C_{159}H_{254}N_{44}O_{56}S_2$	[1489-1507]	X	X	
282	939.94423	939.9521	4	$C_{159}H_{254}N_{44}O_{57}S_2$	[1489-1507] [9)]		X	
283	906.9176	906.9272	6	$C_{228}H_{363}N_{65}O_{81}S_4$	[1475-1507] [6,8)]		H	
284	932.2279	932.2358	5	$C_{199}H_{302}N_{58}O_{68}S_2$	[1490-1520] [5)]		X	**K1507**
285	1046.2809	1046.2888	5	$C_{223}H_{340}N_{64}O_{78}S_2$	[1490-1520]	X	X	
286	1243.5800	1243.5879	6	$C_{328}H_{484}N_{92}O_{105}S_2$	[1490-1537]		X	
287	1066.0686	1066.0764	7			X	X	
288	932.9350	932.9429	8				X	
289	1068.3535	1068.3615	7	$C_{328}H_{484}N_{92}O_{106}S_2$	[1490-1537] [9)]		X	
290	934.9344	934.9422	8				X	
291	875.0674	875.0770	6	$C_{223}H_{342}N_{64}O_{79}S_2$	[1490-1520] [6)]		H	
292	845.6893	845.6972	7	$C_{260}H_{386}N_{78}O_{80}S$	[1508-1546] [5)]		X	**K1537**
293	967.71083	967.7187	4	$C_{169}H_{255}N_{49}O_{54}S$	[1523-1545] [5)]		X	
294	1110.2846	1110.2849	4	$C_{193}H_{293}N_{55}O_{64}S_1$	[1523-1545]	X	X	
295	888.4303	888.4295	5			X	X	
296	892.0252	892.0316	5	$C_{193}H_{295}N_{55}O_{65}S_1$	[1523-1545] [6)]		H	
297	743.5210	743.5276	6				H	
298	716.3195	716.3256	3	$C_{84}H_{139}N_{29}O_{33}S_2$	[1574-1583] [5,8)]	X	X	**K1581**
299	680.0560	680.0624	4	$C_{108}H_{177}N_{35}O_{43}S_2$	[1574-1583] [8)]	X		
300	863.4113	863.4192	5	$C_{190}H_{290}N_{50}O_{61}S_2$	[1582-1605]		X	**K1583**
301	719.6773	719.6840	6				X	
302	866.6103	866.6182	5	$C_{190}H_{290}N_{50}O_{62}S_2$	[1582-1605] [9)]		X	
303	722.3497	722.3498	6			X	X	
304	850.2521	850.2492	6	$C_{227}H_{343}N_{59}O_{71}S_2$	[1584-1614]	X	X	**K1605**
305	728.9212	728.9290	7				X	
306	609.0539	609.0618	4	$C_{108}H_{169}N_{29}O_{33}S$	[1603-1614] [5)]		X	
307	601.4961	601.504	5	$C_{132}H_{207}N_{35}O_{43}S$	[1603-1614]		X	
308	1126.5703	1126.5703	3	$C_{150}H_{233}N_{41}O_{46}S_1$	[1606-1627] [5)]	X	X	**K1614**
309	845.1788	845.1797	4			X	X	
310	676.3446	676.3453	5			X	X	
311	1316.6591	1316.6586	3	$C_{174}H_{271}N_{47}O_{56}S_1$	[1606-1627]	X	X	
312	987.7473	987.7459	4			X	X	
313	790.3967	790.3983	5				X	
314	658.8326	658.8332	6			X	X	
315	849.6740	849.6823	4	$C_{150}H_{235}N_{41}O_{47}S_1$	[1606-1627] [5,6)]		H	
316	679.9392	679.9474	5				H	
317	793.9929	794.0004	5	$C_{174}H_{273}N_{47}O_{57}S_1$	[1606-1627] [6)]		H	
318	661.8275	661.8350	6				H	
319	701.3513	701.3516	4	$C_{117}H_{196}N_{32}O_{45}S_1$	[1671-1681]	X	X	**K1671**
320	886.44257	886.4504	3	$C_{114}H_{185}N_{33}O_{38}S$	[1672-1685] [5)]		X	**K1681**
321	665.08193	665.0898	4			X	X	
322	1076.5309	1076.5388	3	$C_{138}H_{223}N_{39}O_{48}S$	[1672-1685]		X	
323	807.6510	807.6560	4			X	X	
324	646.3195	646.3264	5			X	X	
325	929.1409	929.1488	3	$C_{120}H_{197}N_{35}O_{39}S_1$	[1672-1686] [5)]		X	

326	697.1057	697.1135	4				X	
327	557.8934	557.8924	5			X	X	
328	839.6788	839.6797	4	$C_{144}H_{235}N_{41}O_{49}S_1$	[1672-1686]	X	X	
329	671.9458	671.9454	5			X	X	
330	560.1146	560.1224	6				X	
331	566.6155	566.6234	3	$C_{73}H_{116}N_{24}O_{21}S$	[1681-1685] 5)		X	
332	454.4223	454.4302	5	$C_{97}H_{154}N_{30}O_{31}S$	[1681-1685]		X	
333	669.5844	669.5925	4	$C_{114}H_{187}N_{33}O_{39}S$	[1672-1685] 5,6)		H	
334	535.8675	535.8755	5				H	
335	812.1517	812.1587	4	$C_{138}H_{225}N_{39}O_{49}S$	[1672-1685] 6)		H	
336	561.4871	561.4945	5	$C_{120}H_{199}N_{35}O_{40}S_1$	[1672-1686] 5,6)		H	
337	675.5407	675.5475	5	$C_{144}H_{237}N_{41}O_{50}S_1$	[1672-1686] 6)		H	
338	563.1172	563.1242	6				H	
339	832.7459	832.7450	3	$C_{108}H_{170}N_{30}O_{36}S_1$	[1738-1749] 5)	X	X	
340	1022.8323	1022.8333	3	$C_{132}H_{208}N_{36}O_{46}S_1$	[1738-1749]	X		**K1748**
341	767.3778	767.3770	4			X	X	
342	614.1044	614.1031	5			X	X	
343	656.9231	656.9305	5	$C_{148}H_{222}N_{40}O_{43}S$	[1779-1792]	X	X	
344	1096.2967	1096.2948	4	$C_{198}H_{297}N_{51}O_{60}S_1$	[1764-1792] 5)		X	
345	877.2378	877.2374	5			X	X	
346	1238.8531	1238.861	4	$C_{222}H_{335}N_{57}O_{70}S_1$	[1764-1792]		X	
347	991.2921	991.2903	5			X	X	
348	826.243	826.2433	6			X	X	**K1784**
349	708.3467	708.3525	7				X	
350	880.8295	880.8395	5	$C_{198}H_{299}N_{51}O_{61}S_1$	[1764-1792] 5,6)		H	
351	994.8839	994.8925	5	$C_{222}H_{337}N_{57}O_{71}S_1$	[1764-1792] 6)		H	
352	829.2366	829.2451	6				H	
353	710.9171	710.9254	7				H	
354	1016.7317	1016.7396	4	$C_{177}H_{271}N_{47}O_{61}S$	[1785-1806]		X	
355	924.6497	924.6493	5	$C_{204}H_{308}N_{54}O_{67}S_1$	[1785-1816] 5)		X	
356	1298.1180	1298.1260	4	$C_{228}H_{346}N_{60}O_{77}S_1$	[1785-1816]		X	
357	1038.6979	1038.7023	5			X		**K1792**
358	865.7516	865.7516	6			X	X	
359	817.1853	817.1953	5	$C_{177}H_{273}N_{47}O_{62}S$	[1785-1806]		H	
360	868.7477	868.7550	6	$C_{228}H_{348}N_{60}O_{78}S_1$	[1785-1816]		H	
361	794.3679	794.3757	2	$C_{64}H_{106}N_{20}O_{25}S$	[1898-1903] 5)		X	
362	720.0002	720.0081	3	$C_{88}H_{144}N_{26}O_{35}S$	[1898-1903]		X	
363	886.0734	886.0813	3	$C_{108}H_{178}N_{34}O_{38}S_3$	[1898-1912] 5,8)		X	
364	664.8123	664.8129	4			X	X	**K1902**
365	668.8051	668.8116	4	$C_{108}H_{178}N_{34}O_{39}S_3$	[1898-1912] 5,8,9)	X		
366	807.3787	807.3792	4	$C_{132}H_{216}N_{40}O_{48}S_3$	[1898-1912] 8)	X	X	
367	646.1041	646.1049	5			X	X	
368	649.3046	649.3039	5	$C_{132}H_{216}N_{40}O_{49}S_3$	[1898-1912] 8,9)	X		
369	889.7416	889.7495	3	$C_{110}H_{179}N_{33}O_{38}S_3$	[1903-1916] 5,8)		X	
370	667.5562	667.5641	4				X	**K1912**
371	810.1289	810.1303	4	$C_{134}H_{217}N_{39}O_{48}S_3$	[1903-1916] 8)	X	X	
372	648.3060	648.3058	5			X	X	

373	814.1230	814.1291	4	$C_{134}H_{217}N_{39}O_{49}S_3$	[1903-1916] [8,9]	X		
374	651.4969	651.5048	5				X	
375	619.6306	619.6385	3	$C_{77}H_{129}N_{23}O_{26}S_2$	[1910-1916] [5]		X	
376	607.5392	607.5471	4	$C_{101}H_{167}N_{29}O_{36}S_2$	[1910-1916]		X	
377	611.5381	611.5458	4	$C_{101}H_{167}N_{29}O_{37}S_2$	[1910-1916] [9]		X	
378	941.1236	941.1259	3	$C_{126}H_{189}N_{33}O_{39}S_1$	[1913-1928] [5]		X	**K1916**
379	706.0885	706.0964	4				X	
380	1131.2161	1131.2142	3	$C_{150}H_{227}N_{39}O_{49}S_1$	[1913-1928]	X	X	
381	848.6628	848.6626	4			X	X	
382	679.1238	679.1317	5				X	
383	1137.2104	1137.2177	3	$C_{150}H_{229}N_{39}O_{50}S_1$	[1913-1928] [6]		H	
384	853.1578	853.1652	4				H	
385	682.7263	682.7338	5				H	
386	842.0769	842.0733	3	$C_{111}H_{166}N_{32}O_{34}S_1$	[1917-1929] [5]	X	X	**K1928**
387	1032.1610	1032.1616	3	$C_{135}H_{204}N_{38}O_{44}S_1$	[1917-1929]	X		
388	774.3732	774.3732	4			X	X	
389	1082.1802	1082.1881	3	$C_{143}H_{214}N_{40}O_{45}S$	[1917-1935] [5]		X	
390	954.4606	954.4592	4	$C_{167}H_{252}N_{46}O_{55}S_1$	[1917-1935]	X	X	
391	763.7697	763.7690	5			X	X	
392	725.5295	725.5355	5	$C_{154}H_{231}N_{45}O_{55}S$	[1929-1944]	X		**K1935**
393	604.7730	604.7809	6				X	
394	899.4106	899.4185	7	$C_{278}H_{406}N_{72}O_{92}S_2$	[1929-1967]		X	
395	787.1093	787.1171	8				X	
396	725.0758	725.0759	4	$C_{124}H_{181}N_{35}O_{44}S_1$	[1930-1944] [5]	X	X	
397	867.6415	867.6421	4	$C_{148}H_{219}N_{41}O_{54}S_1$	[1930-1944]	X	X	
398	694.3154	694.3152	5			X	X	
399	622.6776	622.6855	5	$C_{134}H_{197}N_{37}O_{47}S$	[1933-1944]		X	
400	729.5714	729.5786	4	$C_{124}H_{183}N_{35}O_{45}S_1$	[1930-1944] [5,6]		H	
401	583.8571	583.8644	5				H	
402	697.9094	697.9174	5	$C_{148}H_{221}N_{41}O_{55}S_1$	[1930-1944] [6]		H	
403	581.7579	581.7658	6				H	
404	1022.4760	1022.4727	5	$C_{221}H_{331}N_{59}O_{77}S_2$	[1945-1974]	X	X	**K1967**
405	680.9995	681.0074	3	$C_{90}H_{141}N_{23}O_{29}S$	[2023-2030] [5]	X	X	**K2025**
406	653.5659	653.5737	4	$C_{114}H_{179}N_{29}O_{39}S$	[2023-2030]		X	
407	989.9914	989.9993	2	$C_{85}H_{139}N_{23}O_{29}S_1$	[2026-2033] [5]		X	**K2030**
408	660.3355	660.3355	3			X	X	
409	850.4239	850.4238	3	$C_{109}H_{177}N_{29}O_{39}S_1$	[2026-2033]	X	X	
410	638.0701	638.0698	4			X	X	
411	856.4190	856.4273	3	$C_{109}H_{179}N_{29}O_{40}S_1$	[2026-2033] [6]		H	
412	736.1038	736.1130	4	$C_{124}H_{205}N_{33}O_{45}S_2$	[2026-2036] [6]		H	
413	866.9178	866.9220	2	$C_{71}H_{121}N_{21}O_{25}S_2$	[2031-2036] [5]	X		**K2033**
414	578.2851	578.2839	3			X		
415	583.6077	583.6156	3	$C_{71}H_{121}N_{21}O_{26}S_2$	[2031-2036] [5,9]	X	X	
416	768.3729	768.3723	3	$C_{95}H_{159}N_{27}O_{35}S_2$	[2031-2036]	X	X	
417	576.5322	576.5312	4			X	X	
418	773.7045	773.7039	3	$C_{95}H_{159}N_{27}O_{36}S_2$	[2031-2036] [9]	X		
419	580.5301	580.5299	4			X	X	

420	981.1381	981.1481	3	$C_{124}H_{205}N_{33}O_{45}S_2$	[2026-2036] [6)]		H	
421	736.1038	736.1130	4				H	
422	589.0829	589.0920	5				H	
423	744.0252	744.0251	3	$C_{91}H_{152}N_{28}O_{33}S_2$	[2034-2038]		X	**K2036**
424	558.2705	558.2708	4				X	
425	881.75134	881.7568	3	$C_{113}H_{179}N_{31}O_{38}S_2$	[2034-2046] [5)]	X		
426	661.5690	661.5695	4			X	X	
427	1071.8372	1071.8451	3	$C_{137}H_{217}N_{37}O_{48}S_2$	[2034-2046]		X	
428	804.1359	804.1358	4			X	X	
429	643.5099	643.5102	5			X	X	
430	808.1352	808.1345	4	$C_{137}H_{217}N_{37}O_{49}S_2$	[2034-2046] [9)]		X	
431	646.7136	646.7092	5				X	
432	705.6749	705.6828	3	$C_{87}H_{147}N_{27}O_{30}S_2$	[2035-2038]		X	
433	916.1302	916.1381	3	$C_{121}H_{192}N_{34}O_{37}S$	[2037-2050] [5)]		X	**K2046**
434	687.3477	687.3555	4				X	
435	550.0781	550.0860	5				X	
436	1106.2185	1106.2264	3	$C_{145}H_{230}N_{40}O_{47}S_1$	[2037-2050]		X	
437	829.9225	829.9218	4			X	X	
438	664.1386	664.1390	5			X	X	
439	553.6176	553.6171	6			X	X	
440	826.4116	826.4097	3	$C_{109}H_{169}N_{29}O_{35}S_1$	[2039-2050] [5)]	X	X	
441	620.0587	620.0593	4			X	X	
442	762.6245	762.6255	4	$C_{133}H_{207}N_{35}O_{45}S_1$	[2039-2050]	X	X	
443	610.3008	610.3019	5			X	X	
444	834.4177	834.4244	4	$C_{145}H_{232}N_{40}O_{48}S_1$	[2037-2050] [6)]		H	
445	667.7342	667.7411	5				H	
446	556.6118	556.6189	6				H	
447	536.9246	536.9320	3	$C_{67}H_{109}N_{21}O_{23}S$	[2047-2051] [5)]		X	**K2050**
448	684.0007	684.0062	3	$C_{86}H_{140}N_{26}O_{30}S$	[2047-2056] [5)]		X	
449	760.0366	760.0432	3	$C_{96}H_{156}N_{28}O_{34}S$	[2047-2058] [5)]		X	
450	502.4957	502.5016	4	$C_{82}H_{135}N_{29}O_{28}S$	[2071-2079] [5)]	X	X	**K2073**
451	470.2350	470.2410	4	$C_{77}H_{128}N_{28}O_{25}S$	[2072-2079] [5)]	X	X	
452	490.4411	490.4473	5	$C_{101}H_{166}N_{34}O_{35}S$	[2072-2079]	X	X	
453	1045.0104	1045.0125	2	$C_{85}H_{145}N_{27}O_{30}S_2$	[2097-2106] [5)]		X	**K2102**
454	697.0102	697.0109	3			X	X	
455	523.00228	523.0101	4			X	X	
456	702.3435	702.3425	3	$C_{85}H_{145}N_{27}O_{31}S_2$	[2097-2106] [5,9)]	X	X	
457	887.0999	887.0992	3	$C_{109}H_{183}N_{33}O_{40}S_2$	[2097-2106]	X	X	
458	665.5765	665.5764	4			X	X	
459	532.6548	532.6627	5				X	
460	892.4281	892.4308	3	$C_{109}H_{183}N_{33}O_{41}S_2$	[2097-2106] [9)]	X	X	
461	669.5761	669.5751	4			X	X	
462	658.6636	658.6686	3	$C_{81}H_{140}N_{26}O_{27}S_2$	[2098-2106] [5)]	X		
463	636.8118	636.8196	4	$C_{105}H_{178}N_{32}O_{37}S_2$	[2098-2106]	X	X	
464	640.8105	640.8184	4	$C_{105}H_{178}N_{32}O_{38}S_2$	[2098-2106] [9)]		X	
465	703.0065	703.0144	3	$C_{85}H_{147}N_{27}O_{31}S_2$	[2097-2106] [5,6)]		H	
466	527.5049	527.5128	4				H	

467	893.0948	893.1027	3	$C_{109}H_{185}N_{33}O_{41}S_2$	[2097-2106] [6)]		H	
468	670.0711	670.0790	4				H	
469	536.2569	536.2648	5				H	
470	674.0689	674.0778	4	$C_{109}H_{185}N_{33}O_{42}S_2$	[2097-2106] [6,9)]		H	
471	539.4551	539.4637	5				H	
472	1001.4974	1001.4947	5	$C_{224}H_{344}N_{56}O_{68}S_3$	[2154-2183]	X	X	**K2179**
473	828.60706	828.6136	5	$C_{185}H_{284}N_{48}O_{56}S_2$	[2161-2183]	X		
474	1004.4886	1004.4943	3	$C_{131}H_{207}N_{33}O_{46}S$	[2180-2192]		X	**K2183**
475	1107.8684	1107.8683	3	$C_{151}H_{221}N_{37}O_{46}S_1$	[2180-2198] [5)]		X	
476	973.7210	973.7194	4	$C_{175}H_{259}N_{43}O_{56}S_1$	[2180-2198]	X	X	
477	1095.0389	1095.0381	4	$C_{199}H_{294}N_{50}O_{60}S_1$	[2180-2208] [5)]		X	
478	1237.6053	1237.6044	4	$C_{223}H_{332}N_{56}O_{70}S_1$	[2180-2208]		X	
479	1471.7151	1471.7148	3	$C_{202}H_{294}N_{50}O_{60}S_1$	[2184-2212] [5)]		X	**K2208**
480	1104.0413	1104.0381	4				X	
481	1246.6050	1246.6044	4	$C_{226}H_{332}N_{56}O_{70}S_1$	[2184-2212]	X	X	
482	997.4853	997.4850	5			X	X	
483	831.4113	831.4055	6				X	
484	1035.1693	1035.1771	3	$C_{135}H_{211}N_{37}O_{45}S$	[2199-2212]	X	X	
485	776.6325	776.6348	4			X	X	
486	887.0268	887.0342	5	$C_{202}H_{296}N_{50}O_{61}S_1$	[2184-2212] [5,6)]		H	
487	1251.0996	1251.1071	4	$C_{226}H_{334}N_{56}O_{71}S_1$	[2184-2212] [6)]		H	
488	834.3997	834.4073	6				H	
489	800.3833	800.3820	3	$C_{102}H_{159}N_{29}O_{36}S_1$	[2209-2220] [5)]	X	X	**K2212**
490	600.5363	600.5384	4			X		
491	990.4624	990.4703	3	$C_{126}H_{197}N_{35}O_{46}S_1$	[2209-2220]		X	
492	743.1045	743.1046	4			X	X	
493	594.6789	594.6853	5			X		
494	605.0334	605.0411	4	$C_{102}H_{161}N_{29}O_{37}S_1$	[2209-2220] [5,6)]		H	
495	747.5998	747.6073	4	$C_{126}H_{199}N_{35}O_{47}S_1$	[2209-2220] [6)]		H	
496	790.0796	790.0798	3	$C_{107}H_{166}N_{30}O_{29}S_1$	[2299-2309] [5)]	X	X	**K2308**
497	980.1602	980.1681	3	$C_{131}H_{204}N_{36}O_{39}S_1$	[2299-2309]		X	
498	735.3780	735.3780	4			X	X	
499	986.1629	986.1716	3	$C_{131}H_{206}N_{36}O_{40}S_1$	[2299-2309] [6)]		H	
500	770.3677	770.3755	5	$C_{159}H_{263}N_{51}O_{52}S_4$	[2309-2326] [8,9)]		X	**K2311**
501	496.2516	496.2594	4	$C_{84}H_{136}N_{30}O_{24}S$	[2310-2316] [5)]		X	
502	397.2013	397.2091	5				X	
503	638.8247	638.8257	4	$C_{108}H_{174}N_{36}O_{34}S_1$	[2310-2316]	X	X	
504	511.2557	511.2621	5			X		
505	599.7925	599.8004	4	$C_{102}H_{162}N_{32}O_{33}S$	[2311-2316]	X	X	
506	480.0340	480.0419	5			X	X	
507	709.0807	709.0811	4	$C_{117}H_{189}N_{37}O_{37}S_4$	[2312-2326] [5,8)]	X	X	**K2316**
508	681.5115	681.5193	5	$C_{141}H_{227}N_{43}O_{47}S_4$	[2312-2326] [8)]		X	
509	568.0941	568.1008	6			X		
510	684.7105	684.7184	5	$C_{141}H_{227}N_{43}O_{48}S_4$	[2312-2326] [8,9)]		X	
511	1012.9605	1012.9593	4	$C_{172}H_{262}N_{52}O_{52}S_5$	[2317-2342] [5,8)]	X		**K2326**
512	810.5692	810.5690	5			X	X	
513	675.6343	675.6422	6				X	

514	813.7601	813.7680	5	$C_{172}H_{262}N_{52}O_{53}S_5$	[2317-2342] [5,8,9]		X	
515	1155.5272	1155.5255	4	$C_{196}H_{300}N_{58}O_{62}S_5$	[2317-2342] [8]	X	X	
516	924.6141	924.6220	5				X	
517	927.8157	927.8210	5	$C_{196}H_{300}N_{58}O_{63}S_5$	[2317-2342] [8,9]		X	
518	773.3455	773.3521	6				X	
519	814.1612	814.1711	5	$C_{172}H_{264}N_{52}O_{53}S_5$	[2317-2342] [8,6,5]		H	
520	678.6344	678.6439	6				H	
521	928.2170	928.2241	5	$C_{196}H_{302}N_{58}O_{63}S_5$	[2317-2342] [8,6]		H	
522	773.6809	773.6880	6				H	
523	663.2979	663.3052	7				H	
524	547.5096	547.5175	4	$C_{88}H_{147}N_{29}O_{34}S$	[2381-2385]		X	**K2381**
525	894.8991	894.9070	4	$C_{148}H_{234}N_{42}O_{55}S_3$	[2408-2426] [8]		X	
526	793.9553	793.9556	5	$C_{168}H_{253}N_{49}O_{55}S_4$	[2408-2433] [5,8]		X	
527	908.00072	908.0086	5	$C_{192}H_{291}N_{55}O_{65}S_4$	[2408-2433] [8]		X	
528	756.8403	756.8418	6				X	
529	726.6587	726.6653	6	$C_{187}H_{280}N_{54}O_{59}S_4$	[2408-2436] [5,8]	X		
530	985.8549	985.8499	5	$C_{211}H_{318}N_{60}O_{69}S_4$	[2408-2436] [8]	X		
531	821.7090	821.7095	6			X	X	**K2425**
532	704.4586	704.4664	7				X	
533	989.0410	989.0488	5	$C_{211}H_{318}N_{60}O_{70}S_4$	[2408-2436] [8,9]		X	
534	824.3687	824.3754	6			X	X	
535	989.0410	989.0488	5		[2408-2436] [8,9]		X	
536	824.3675	824.3754	6			X	X	
537	706.7446	706.7514	7			X	X	
538	707.0314	707.0394	7	$C_{211}H_{320}N_{60}O_{70}S_4$	[2408-2436] [6,8]		H	
539	857.3980	857.4059	4	$C_{151}H_{224}N_{42}O_{46}S_2$	[2426-2444] [5]		X	
540	686.1259	686.1263	5			X	X	
541	800.1714	800.1793	5	$C_{175}H_{262}N_{48}O_{56}S_2$	[2426-2444]		X	
542	803.3718	803.3782	5	$C_{175}H_{262}N_{48}O_{57}S_2$	[2426-2444] [9]	X	X	**2436**
543	780.0558	780.0553	3	$C_{102}H_{160}N_{28}O_{33}S_1$	[2434-2444] [5]	X	X	
544	970.1357	970.1436	3	$C_{126}H_{198}N_{34}O_{43}S_1$	[2434-2444]	X		
545	727.8608	727.8596	4			X	X	
546	1369.6661	1369.6655	3	$C_{184}H_{276}N_{46}O_{59}S_1$	[2437-2463] [5]		X	
547	1027.5017	1027.5011	4			X	X	
548	822.1946	822.2025	5				X	
549	1559.7536	1559.7539	3	$C_{208}H_{314}N_{52}O_{69}S_1$	[2437-2463]	X	X	
550	1170.0685	1170.0674	4			X	X	
551	936.2565	936.2554	5			X	X	**K2444**
552	1031.9957	1032.0038	4	$C_{184}H_{278}N_{46}O_{60}S_1$	[2437-2463] [5,6]		H	
553	825.7966	825.8046	5				H	
554	1174.5621	1174.5699	4	$C_{208}H_{316}N_{52}O_{70}S_1$	[2437-2463] [6]		H	
555	939.8496	939.8575	5				H	
556	783.3747	783.3826	6				H	
557	912.09847	912.1064	3	$C_{120}H_{184}N_{30}O_{41}S$	[2456-2465]		X	**K2463**
558	891.7765	891.7770	3	$C_{110}H_{185}N_{33}O_{42}S_1$	[2508-2522] [5]	X	X	
559	1081.8637	1081.8654	3	$C_{134}H_{223}N_{39}O_{52}S_1$	[2508-2522]	X	X	**K2508**
560	811.6508	811.6509	4			X	X	

561	946.4485	946.4562	2	$C_{81}H_{130}N_{22}O_{26}S_2$	[2574-2580] [5)]		X	**K2577**
562	710.14588	710.1537	5	$C_{155}H_{240}N_{46}O_{46}S_2$	[2719-2739] [5,8)]		X	**K2735**
563	824.2070	824.2067	5	$C_{179}H_{278}N_{52}O_{56}S_2$	[2719-2739] [8)]	X	X	
564	686.99905	687.0669	6				X	
565	807.6505	807.6491	4	$C_{140}H_{219}N_{41}O_{43}S_2$	[2721-2739] [5,8)]	X	X	
566	760.3733	760.3738	5	$C_{164}H_{257}N_{47}O_{53}S_2$	[2721-2739] [8)]	X	X	
567	688.7094	688.7144	3	$C_{90}H_{154}N_{26}O_{27}S$	[2731-2739] [5)]	X	X	
568	878.7948	878.8027	3	$C_{114}H_{192}N_{32}O_{37}S$	[2731-2739]		X	
569	659.3468	659.3540	4				X	
570	838.3967	838.4046	3	$C_{108}H_{169}N_{29}O_{38}S$	[2736-2743]	X	X	**K2739**
571	729.3596	729.3607	3	$C_{93}H_{148}N_{28}O_{31}S_1$	[2736-2745] [5)]	X	X	
572	547.2690	547.2725	4				X	
573	919.4480	919.4490	3	$C_{117}H_{186}N_{34}O_{41}S_1$	[2736-2745]	X	X	
574	689.8375	689.8387	4			X	X	
575	552.0725	552.0725	5			X	X	
576	422.4539	422.4617	4	$C_{68}H_{115}N_{23}O_{25}S$	[2791-2795] [5)]		X	**K2792**
577	565.0201	565.0280	4	$C_{92}H_{153}N_{29}O_{35}S$	[2791-2795]		X	
578	710.3357	710.3363	3	$C_{86}H_{141}N_{27}O_{34}S_1$	[2792-2795]		X	
579	533.0034	533.0042	4				X	
580	537.4983	537.5068	4	$C_{86}H_{143}N_{27}O_{35}S_1$	[2792-2795] [6)]		H	
581	430.1986	430.2070	5				H	
582	989.0093	989.0097	2	$C_{86}H_{141}N_{23}O_{28}S_1$	[2847-2854] [5)]	X	X	**K2851**
583	659.6765	659.6757	3			X	X	
584	849.7626	849.7640	3	$C_{110}H_{179}N_{29}O_{38}S_1$	[2847-2854]	X	X	
585	637.5747	637.5750	4			X	X	
586	665.6699	665.6793	3	$C_{86}H_{143}N_{23}O_{29}S_1$	[2847-2854] [5,6)]		H	
587	642.0691	642.0776	4	$C_{110}H_{181}N_{29}O_{39}S_1$	[2847-2854] [6)]		H	
588	513.8553	513.8636	5				H	
589	608.6244	608.6323	6	$C_{154}H_{248}N_{42}O_{58}S$	[2916-2934]		X	**K2929**
590	676.6543	676.6622	3	$C_{84}H_{138}N_{24}O_{32}S$	[2989-2992]		X	**K2991**
591	618.4613	618.4692	6	$C_{165}H_{245}N_{45}O_{51}S$	[2989-3006]		X	
592	742.5957	742.6019	4	$C_{124}H_{195}N_{39}O_{42}S_2$	[3027-3038]	X	X	**K3031**
593	594.2767	594.2831	5			X	X	
594	495.3960	495.4039	6				X	
595	557.0317	557.0396	4	$C_{93}H_{157}N_{29}O_{32}S$	[3124-3128]		X	**K3126**
596	423.2154	423.2237	5	$C_{88}H_{150}N_{28}O_{30}S$	[3127-3130]		X	**K3129**
597	622.5556	622.5634	4	$C_{106}H_{171}N_{31}O_{36}S$	[3129-3136]		X	**K3130**
598	498.2444	498.2523	5				X	
599	787.0449	787.0503	3	$C_{100}H_{159}N_{29}O_{35}S_1$	[3130-3136]	X		
600	590.5405	590.5397	4			X	X	
601	594.6797	594.6875	5	$C_{125}H_{197}N_{37}O_{45}S$	[3162-3174]	X	X	**K3165**
602	898.0106	898.0134	5	$C_{193}H_{289}N_{53}O_{67}S_2$	[3227-3252]	X	X	**K3244**
603	772.6464	772.6543	4	$C_{137}H_{219}N_{37}O_{42}S$	[3303-3321] [5)]		X	**K3317**
604	915.2127	915.2205	4	$C_{161}H_{257}N_{43}O_{52}S_1$	[3303-3321]		X	
605	732.3785	732.3780	5			X		
606	708.3740	708.3790	4	$C_{127}H_{204}N_{34}O_{37}S$	[3305-3321] [5)]	X	X	
607	680.9523	680.9578	5	$C_{151}H_{242}N_{40}O_{47}S$	[3305-3321]	X		

608	546.2803	546.2881	4	$C_{92}H_{156}N_{28}O_{31}S$	[3322-3326]		X	**K3325**
609	778.68202	778.6873	3	$C_{100}H_{148}N_{28}O_{35}S$	[3375-3386] [5)]	X	X	**K3385**
610	968.77071	968.7756	3	$C_{124}H_{186}N_{34}O_{45}S$	[3375-3386]	X	X	
611	726.82713	726.8336	4			X	X	
612	806.1199	806.1245	4	$C_{135}H_{209}N_{41}O_{47}S_2$	[3375-3394] [5,8)]	X		

[1)] Numbers inside brackets correspond to the position of the proteolytic peptide within the sequence of KLH2. All peptides from KLH2 shown in this table are linked to (C^1-K^{16}) fragment of Cys^1pP0, except those peptides where it is specified if they are linked to (C^1-K^{11}), (C^1-K^{14}) or (C^1-K^{17}) fragment of Cys^1pP0.
[2)] Identification of type 2 peptides in the KLH2-Cys^1pP0 conjugate using pLink2 software [2].
[3)] Identification of type 2 peptides in the KLH2-Cys^1pP0 conjugate using Kojak software [3].
[4)] Indicates the position where the peptide Cys^1pP0 is added by the Michael addition to the free amino groups in the Lys residues or *N*-terminus of the KLH2.
[5)] Peptide from KLH2 linked to (C^1-K^{11}) fragment of Cys^1pP0
[6)] Identification of type 2 peptides with the hydrolyzed linker
[7)] Peptide from KLH2 linked to (C^1-K^{17}) fragment of Cys^1pP0
[8)] Carbamidomethylation of Cys
[9)] Met→ Met sulfoxide
[10)] Peptide from KLH2 linked to (C^1-K^{14}) fragment of Cys^1pP0

Table S8. Identification of type 2 peptides derived from the proteolytic digestion of KLH2-Cys[1]pP0 conjugate with trypsin using the MED-FASP method [4]. Type 2 peptides were identified using transcyclized linker.

#	Assignment [1)]	z	Conjugation site [2)]	m/z theor	m/z exp	Error (ppm)	RT1 [3)]	RT2 [4)]	Ion [5)]
1	[1-7]-(C1-K16)	4	Nterm	596.8019	596.8028	-1.51	15.29	23.19	3
2	[7-22]-(C1-K11)	3	K7	915.4508	915.4522	-1.57	39.50	39.75	2
3	[7-22]-(C1-K16)	4		829.4060	829.4074	-1.63	36.59	36.83	3
4	[23-55]-(C1-K11) [6)]	5	K52	941.0257	941.0270	-1.45	39.02	-	-
5	[23-55]-(C1-K16) [6)]	6		879.4001	879.4014	-1.42	37.23	-	3
6		5		1055.0785	1055.0801	-1.48	37.23	-	3
7	[128-136]-(C1-K11)	3	K135	683.0135	683.0146	-1.56	34.11	34.52	1,2
8		2		1024.0164	1024.0180	-1.51	34.11	-	1
9	[128-136]-(C1-K16)	4		655.0781	655.0791	-1.53	31.48	31.86	1,3
10		3		873.1015	873.1028	-1.57	31.47	31.86	1,3
11	[136-139] -(C1-K16)	4	K136	515.5020	515.5028	-1.50	12.41	12.68	1,3
12	[140-156]-(C1-K11)	5	K148	601.2984	601.2993	-1.50	29.75	-	-
13	[140-156]-(C1-K16)	6		596.2940	596.2949	-1.45	28.34	-	3
14	[145-156]-(C1-K11)	4		612.3062	612.3071	-1.39	22.63	23.05	1,2
15		5		490.0465	490.0472	-1.43	22.63	23.06	1
16	[145-156]-(C1-K16)	6		503.5840	503.5848	-1.56	21.96	22.29	1,3
17		4		754.8722	754.8733	-1.42	21.96	22.29	1,3
18		5		604.0993	604.1002	-1.46	21.98	22.30	1,2,3
19	[230-252]-(C1-K11) [6)]	5	K231	724.7275	724.7285	-1.41	35.68	35.87	2
20		4		905.6574	905.6587	-1.44	35.68	-	2
21	[230-252]-(C1-K16) [6,7)]	6		701.8174	701.8184	-1.38	30.13	-	3
22	[230-252]-(C1-K16) [6)]	5		838.7803	838.7815	-1.43	33.62	33.78	3

23	[230-261]-(C1-K11) [6)]	6		775.0263	775.0274	-1.46	43.39	-	2
24		5		929.8300	929.8314	-1.46	43.37	-	2
25	[230-261]-(C1-K16) [6)]	6		870.0703	870.0716	-1.48	41.44	-	2,3
26		7		745.9185	745.9196	-1.49	41.44	-	3
27	[300-304]-(C1-K11)	3	K302	524.5911	524.5919	-1.40	12.47	12.88	1
28	[300-304]-(C1-K16)	4		536.2612	536.2620	-1.59	13.72	14.09	1,3
29		3		714.6791	714.6801	-1.45	13.72	14.09	1,3
30	[340-358]-(C1-K11)	3	K353	1063.8345	1063.8360	-1.41	54.31	-	2
31		4		798.1278	798.1290	-1.44	54.31	-	2
32	[340-358]-(C1-K16) [7)]	4		944.6925	944.6939	-1.48	52.26	53.55	3
33	[340-358]-(C1-K16)	4		940.6938	940.6952	-1.46	53.87	-	2,3
34		3		1253.9225	1253.9243	-1.44	53.86	-	3
35		5		752.7566	752.7577	-1.46	53.90	-	3
36	[400-414]-(C1-K11)	5	K409	546.4802	546.4810	-1.54	20.55	20.72	-
37	[400-427]-(C1-K16)	7		659.6343	659.6353	-1.54	31.59	31.80	3
38		6		769.4054	769.4066	-1.52	31.59	31.78	3
39	[407-427]-(C1-K11)	5		642.7381	642.7390	-1.46	33.99	34.20	-
40	[407-427]-(C1-K16)	6		630.8270	630.8280	-1.56	32.25	32.46	3
41	[410-427]-(C1-K11)	4	K414	729.1246	729.1257	-1.44	38.01	38.20	2
42	[410-427]-(C1-K16)	5		697.5540	697.5551	-1.52	35.59	35.80	3
43		4		871.6906	871.6919	-1.46	35.60	35.80	3
44	[428-442]-(C1-K11)	3	K428	922.1108	922.1122	-1.52	36.57	36.85	2
45	[428-442]-(C1-K16)	4		834.4010	834.4023	-1.59	34.01	34.32	3
46	[443-447]-(C1-K11)	3	K443	544.5922	544.5930	-1.35	15.62	16.10	1
47	[443-447]-(C1-K16) [7)]	4		555.2608	555.2616	-1.49	13.45	13.67	3
48		4		551.2621	551.2629	-1.45	16.19	16.60	1,3
49	[443-452]-(C1-K16)	4		713.3335	713.3346	-1.51	28.34	28.63	3

50	[448-469]-(C1-K16)	5	K452	812.9870	812.9882	-1.45	36.41	36.58	2,3
51		4		1015.9818	1015.9833	-1.45	36.41	36.58	2,3
52	[448-469]-(C1-K11)	4		873.4158	873.4171	-1.43	38.13	38.66	2
53	[470-478]-(C1-K16) [6)]	5	K476	537.2527	537.2535	-1.45	15.85	16.20	2,3
54		4		671.3140	671.3149	-1.34	15.85	16.19	3
55	[652-656]-(C1-K16)	4	K653	538.2597	538.2605	-1.49	16.06	-	1,3
56	[666-682]-(C1-K11)	3	K669	977.1421	977.1436	-1.54	44.75	44.94	2
57	[703-728]-(C1-K16)	5	K722	948.6266	948.6279	-1.43	51.88	-	3
58		6		790.6901	790.6913	-1.48	51.88	-	3
59	[769-776]-(C1-K16)	4	K771	659.8017	659.8027	-1.44	31.36	-	3
60	[769-776]-(C1-K11)	3		689.3117	689.3126	-1.31	34.22	-	-
61	[826-835]-(C1-K11)	4	K829	525.9931	525.9938	-1.43	34.11	-	-
62	[917-931]-(C1-K11)	4	K917	705.3338	705.3348	-1.42	44.32	44.50	2
63		3		940.1092	940.1105	-1.35	44.29	-	-
64	[917-931]-(C1-K16)	5		678.5214	678.5224	-1.44	41.22	41.38	3
65		4		847.8998	847.9010	-1.44	41.22	41.38	3
66	[1046-1062]-(C1-K11)	4	K1060	787.3945	787.3956	-1.46	50.13	-	-
67	[1063-1077]-(C1-K11) [6)]	3	K1064	884.4082	884.4094	-1.39	30.62	30.92	-
68	[1063-1077]-(C1-K16) [6)]	4		806.1241	806.1252	-1.43	28.60	28.89	3
69	[1078-1096]-(C1-K11)	3	K1078	1046.8424	1046.8440	-1.53	47.37	47.55	-
70		4		785.3838	785.3850	-1.46	47.39	47.55	-
71	[1078-1096]-(C1-K16)	4		927.9497	927.9512	-1.59	44.07	44.26	3
72		3		1236.9304	1236.9323	-1.54	44.08	44.26	3
73	[1078-1103]-(C1-K11)	5		798.9932	798.9944	-1.45	45.85	45.97	-
74		4		998.4895	998.4910	-1.50	45.86	45.97	-
75	[1078-1103]-(C1-K16)	6		761.0396	761.0408	-1.51	43.49	43.64	3
76		5		913.0460	913.0474	-1.47	43.49	43.64	3

77	[1261-1264]-(C1-K16)	3	K1261	700.0158	700.0169	-1.52	16.46	16.89	1,3
78	[1276-1292]-(C1-K11)	3	K1283	983.8296	983.8311	-1.56	45.72	45.85	-
79	[1276-1292]-(C1-K16)	4		880.6902	880.6915	-1.50	42.71	-	3
80		3		1173.9176	1173.9194	-1.56	42.71	-	3
81	[1284-1296]-(C1-K11)	4	K1292	626.5559	626.5568	-1.44	32.61	32.95	-
82	[1336-1366]-(C1-K16)	4	K1349	1261.0936	1261.0956	-1.55	54.08	54.35	2,3
83		5		1009.0765	1009.0780	-1.49	54.08	54.35	2,3
84	[1436-1461]-(C1-K11)	4	K1437	1003.4827	1003.4842	-1.47	53.82	-	2
85	[1436-1461]-(C1-K16)	5		917.0405	917.0419	-1.50	53.41	-	2,3
86		7		655.3169	655.3179	-1.46	53.42	-	3
87	[1472-1488]-(C1-K11) [6)]	6	K1474	524.4108	524.4116	-1.40	27.59	-	-
88	[1474-1488]-(C1-K11) [6)]	5		565.2586	565.2594	-1.42	27.47	-	-
89	[1475-1488]-(C1-K11) [6)]	3	K1475	898.7276	898.7288	-1.37	27.70	28.00	-
90	[1489-1507]-(C1-K11)	3	K1489	1057.5118	1057.5134	-1.48	41.89	42.10	-
91	[1489-1507]-(C1-K16) [7)]	4		939.9506	939.9520	-1.52	35.00	35.25	3
92	[1489-1507]-(C1-K16)	4		935.9518	935.9533	-1.60	38.94	39.14	3
93	[1490-1520]-(C1-K11)	5	K1507	932.2344	932.2357	-1.39	46.37	46.47	-
94	[1490-1520]-(C1-K16)	5		1046.2872	1046.2887	-1.43	44.37	-	3
95	[1523-1545]-(C1-K11)	3	K1537	1289.9537	1289.9556	-1.45	49.31	-	-
96		4		967.7172	967.7186	-1.47	49.31	-	-
97	[1523-1545]-(C1-K16)	5		888.4281	888.4294	-1.51	46.95	-	3
98		4		1110.2832	1110.2848	-1.49	46.96	-	3
99	[1603-1614]-(C1-K11)	4	K1605	609.0608	609.0617	-1.52	41.23	41.50	1
100	[1603-1614]-(C1-K16)	5		601.5030	601.5039	-1.53	38.38	38.60	3
101	[1606-1627]-(C1-K16)	5	K1614	790.3970	790.3982	-1.54	53.89	-	3
102		4		987.7443	987.7459	-1.54	53.88	-	3
103		6		658.8321	658.8331	-1.59	53.90	-	3

104	[1615-1631]-(C1-K11)	4	K1627	709.3612	709.3623	-1.52	46.17	46.32	-
105	[1671-1681]-(C1-K11)	3	K1671	744.7100	744.7112	-1.61	29.75	-	-
106	[1671-1681]-(C1-K16)	4		701.3504	701.3516	-1.68	27.81	28.12	3
107	[1672-1685]-(C1-K16)	5	K1681	646.3253	646.3263	-1.58	41.40	-	3
108		4		807.6547	807.6559	-1.55	41.41	-	3
109		3		1076.5370	1076.5387	-1.55	41.41	-	3
110	[1672-1685]-(C1-K11)	4		665.0887	665.0897	-1.54	40.05	-	2
111		3		886.4490	886.4504	-1.54	44.51	-	-
112	[1686-1689]-(C1-K16)	4	K1686	507.5108	507.5116	-1.58	16.15	16.56	1,3
113	[1738-1749]-(C1-K11)	3	K1748	832.7436	832.7449	-1.56	38.93	39.33	-
114	[1738-1749]-(C1-K16)	4		767.3757	767.3768	-1.50	36.02	36.27	2,3
115		3		1022.8316	1022.8332	-1.56	36.02	36.27	3
116	[1764-1792]-(C1-K16)	6	K1784	826.2419	826.2432	-1.57	53.57	-	3
117		5		991.2888	991.2903	-1.49	53.57	-	3
118	[1785-1806]-(C1-K16)	4	K1792	1016.7379	1016.7395	-1.55	49.56	-	3
119	[1898-1912]-(C1-K11) [6)]	4	K1902	664.8119	664.8129	-1.43	26.51	26.75	1
120		3		886.0799	886.0812	-1.47	26.52	26.75	-
121	[1898-1912]-(C1-K16) [6)]	5		646.1039	646.1048	-1.42	25.14	25.40	1,3
122		4		807.3779	807.3791	-1.46	25.14	25.40	1,3
123	[1913-1928]-(C1-K16)	4	K1916	848.6612	848.6625	-1.56	44.13	44.35	3
124	[1917-1929]-(C1-K11)	3	K1928	842.0720	842.0732	-1.46	39.34	39.60	-
125	[1917-1929]-(C1-K16)	3		1032.1600	1032.1616	-1.52	36.62	-	3
126		4		774.3720	774.3731	-1.45	36.35	36.62	3
127	[1929-1944]-(C1-K11)	5	K1935	611.4816	611.4824	-1.37	28.19	28.50	-
128		4		764.1000	764.1011	-1.44	28.16	28.50	-
129	[1929-1944]-(C1-K16)	6		604.7800	604.7808	-1.35	26.90	27.22	3
130	[1930-1944]-(C1-K11)	4		725.0748	725.0758	-1.41	31.07	31.38	2

131	[1930-1944]-(C1-K16)	4		867.6408	867.6420	-1.44	29.29	29.59	3
132		5		694.3142	694.3152	-1.44	29.30	29.59	3
133	[1945-1974]-(C1-K16)	5	K1967	1022.4710	1022.4725	-1.51	53.76	-	3
134	[1945-1974]-(C1-K11)	4		1135.2709	1135.2725	-1.41	54.04	-	-
135	[2023-2030]-(C1-K11)	3	K2025	681.0062	681.0073	-1.62	29.13	29.55	1,2
136	[2023-2030]-(C1-K16)	4		653.5726	653.5737	-1.61	27.30	27.64	1,3
137	[2026-2033]-(C1-K11)	3	K2030	660.3344	660.3354	-1.51	30.26	30.60	1
138	[2026-2033]-(C1-K16)	4		638.0687	638.0698	-1.65	28.19	28.50	1,3
139	[2031-2036]-(C1-K16)	4	K2033	576.5302	576.5311	-1.56	21.06	21..33	1,3
140	[2034-2038]-(C1-K16)	3	K2036	744.0239	744.0250	-1.52	21.96	22.32	1,3
141		4		558.2699	558.2708	-1.48	21.96	22.32	1,3
142	[2037-2050]-(C1-K16)	5	K2046	664.1379	664.1389	-1.54	35.32	35.55	3
143	[2039-2050]-(C1-K11)	4		620.0582	620.0592	-1.57	37.60	37.87	-
144		3		826.4084	826.4096	-1.49	37.60	37.87	-
145	[2039-2050]-(C1-K16)	4		762.6242	762.6254	-1.57	34.90	35.16	3
146		5		610.3009	610.3019	-1.61	34.90	35.17	1,3
147	[2097-2106]-(C1-K16) [7)]	3	K2102	892.4294	892.4308	-1.53	28.32	28.68	2,3
148		4		669.5740	669.5750	-1.53	28.32	28.68	3
149	[2097-2106]-(C1-K16)	4		665.5753	665.5763	-1.50	35.21	35.57	1,2,3
150		3		887.0978	887.0991	-1.50	35.20	35.58	1,2,3
151	[2097-2106]-(C1-K11) [7)]	3		702.3414	702.3425	-1.52	30.32	30.75	1,2
152	[2097-2106]-(C1-K11)	3		697.0098	697.0108	-1.48	38.37	38.75	1,2
153		2		1045.0107	1045.0123	-1.48	38.37	38.75	2
154	[2154-2183]-(C1-K16)	5	K2179	1001.4931	1001.4946	-1.52	54.21	-	3
155	[2180-2198]-(C1-K11)	3	K2183	1107.8665	1107.8682	-1.47	54.08	-	2
156	[2180-2198]-(C1-K16)	4		973.7178	973.7193	-1.51	53.56	-	2,3
157	[2199-2212]-(C1-K16)	4	K2208	776.6336	776.6348	-1.51	37.61	37.83	3

158		3		1035.1755	1035.1771	-1.55	37.63	37.83	3
159	[2199-2212]-(C1-K11)	3		845.0875	845.0888	-1.50	40.90	41.15	-
160	[2209-2220]-(C1-K11)	3	K2212	800.3807	800.3819	-1.46	28.23	28.55	-
161	[2209-2220]-(C1-K16)	3		990.4687	990.4702	-1.48	26.59	26.90	1,2,3
162		4		743.1034	743.1046	-1.58	26.59	26.90	1,2,3
163	[2299-2309]-(C1-K11)	3	K2308	790.0785	790.0797	-1.48	48.42	48.60	-
164	[2299-2309]-(C1-K16)	4		735.3768	735.3779	-1.53	44.90	45.10	3
165	[2311-2316]-(C1-K11)	4	K2311	457.2334	457.2341	-1.53	10.38	10.99	-
166	[2311-2316]-(C1-K16)	5		480.0411	480.0418	-1.50	12.33	12.52	1,3
167		4		599.7994	599.8004	-1.54	12.33	12.52	1,3
168	[2381-2385]-(C1-K16)	4	K2381	547.5166	547.5174	-1.46	12.58	12.90	1,3
169	[2408-2433]-(C1-K11) 6,7)	5	K2425	797.1534	797.1545	-1.41	45.03	-	-
170	[2408-2433]-(C1-K11) [6)]	5		793.9544	793.9556	-1.44	48.44	-	-
171		4		992.1911	992.1925	-1.39	48.45	-	-
172	[2408-2433]-(C1-K16) [6)]	5		908.0072	908.0085	-1.45	46.00	-	3
173		6		756.8407	756.8417	-1.37	46.04	-	3
174	[2434-2444]-(C1-K11)	3	K2436	780.0540	780.0552	-1.54	42.71	42.93	2
175	[2434-2444]-(C1-K16)	4		727.8585	727.8596	-1.48	39.39	39.60	1,2,3
176		3		970.1420	970.1435	-1.55	39.38	39.60	3
177	[2437-2463]-(C1-K16)	4	K2444	1170.0654	1170.0673	-1.58	53.83	-	2,3
178	[2508-2522]-(C1-K11)	3	K2508	891.7755	891.7769	-1.61	41.67	41.93	2
179	[2508-2522]-(C1-K16)	4		811.6496	811.6509	-1.57	38.76	39.00	2,3
180		3		1081.8635	1081.8652	-1.60	38.78	-	3
181	[262-274]-(C1-K16)	5	K265	612.8805	612.8814	-1.37	23.32	23.58	3
182		4		765.8486	765.8497	-1.47	23.32	23.58	3
183	[262-274]-(C1-K11)	4		623.2826	623.2835	-1.44	24.35	24.73	1,2
184		3		830.7076	830.7087	-1.36	24.35	24.73	-

185	[2721-2739]-(C1-K16) [6)]	5	K2735	760.3726	760.3738	-1.55	36.80	36.95	3
186	[2721-2739]-(C1-K11) [6)]	4		807.6478	807.6491	-1.55	39.06	39.23	-
187	[2736-2745]-(C1-K11)	3	K2739	729.3595	729.3607	-1.55	29.25	29.65	2
188	[2736-2745]-(C1-K16)	4		689.8376	689.8386	-1.52	27.30	27.60	2,3
189		3		919.4475	919.4489	-1.56	27.30	27.60	3
190	[2791-2795]-(C1-K11)	4	K2792	422.4610	422.4616	-1.54	9.62	9.80	1
191	[2791-2795]-(C1-K16)	4		565.0270	565.0279	-1.55	11.34	11.59	1,3
192		4		533.0034	533.0042	-1.41	13.16	13.55	1,3
193	[2792-2795]-(C1-K16)	3		710.3352	710.3362	-1.50	13.16	13.55	1,3
194	[2847-2854]-(C1-K11)	3	K2851	659.6746	659.6757	-1.62	36.71	37.02	1,2
195		2		989.0080	989.0096	-1.62	36.70	37.02	-
196	[2847-2854]-(C1-K16)	3		849.7626	849.7640	-1.61	33.64	33.96	3
197		4		637.5739	637.5750	-1.61	33.65	33.95	1,3
198	[2989-3006]-(C1-K16)	6	K2991	618.4682	618.4691	-1.51	36.38	-	3
199	[3027-3038]-(C1-K16)	5	K3031	594.2822	594.2830	-1.38	19.74	19.94	1,3
200		6		495.4031	495.4038	-1.45	19.75	19.94	3
201		4		742.6008	742.6018	-1.38	19.74	19.94	3
202	[3129-3136]-(C1-K16)	5	K3130	498.2515	498.2522	-1.49	14.84	15.20	3
203		4		622.5624	622.5634	-1.53	14.85	15.20	1,3
204	[3162-3174]-(C1-K16)	5	K3165	594.6866	594.6874	-1.45	23.00	23.35	3
205	[3227-3252]-(C1-K16)	5	K3244	898.0120	898.0133	-1.45	47.41	-	3
206	[3322-3326]-(C1-K16)	4	K3325	546.2872	546.2881	-1.60	20.03	20.35	1,3
207	[3375-3394]-(C1-K16) [6)]	4	K3385	948.6892	948.6906	-1.50	31.30	31.50	3
208	[3375-3394]-(C1-K11) [6)]	4		806.1232	806.1244	-1.49	33.38	33.60	2

[1)] Numbers inside brackets and parentheses correspond to the position of the proteolytic peptide within the sequences of KLH2 and Cys[1]pP0, respectively.

[2] Indicates the position where the peptide Cys[1]pP0 is added by the Michael addition to the free amino groups in the Lys residues or N-terminus of the KLH2.

[3] Retention time of the first peak of type 2 peptides

[4] Retention time of the second peak of type 2 peptides

[5] Type 2 peptides containing the P+71 ion fragment (1), C+80 ion fragment (2), y5 α/β fragment ion (m/z = 589.282, 1+) (3) or not containing any ion fragments (-).

[6] Carbamidomethylation of Cys

[7] Met→ Met sulfoxide

Table S9. Identification of type 2 peptides derived from the proteolytic digestion of KLH2-Cys[1]pP0 conjugate with trypsin using the MED-FASP method [4]. Type 2 peptides were identified using hydrolyzed thiosuccinimide linker.

	Assignment [1)]	z	Conjugation site [2)]	m/z theor.	m/z exp.	Error (ppm)	RT1 [3)]	RT2 [4)]	RT3 [5)]	RT4 [6)]	Ion [7)]
1	[128 - 136]-(C1-K11)	3	(K135)	689.0140	689.0181	-1.60	30.08	-	-	-	-
2	[128 - 136]-(C1-K16)	4		659.5804	659.5814	-1.59	24.03	24.28	-	-	5
3	[145 - 156]-(C1-K11)	4	(K148)	616.8088	616.8094	-1.46	19.64	19.48	20.35	20.55	1,4
4		5		493.6486	493.6493	-1.46	19.64	19.48	20.36	20.55	-
5	[145 - 156]-(C1-K16)	5		604.4014	604.4023	-1.48	19.60	19.43	20.12	20.32	1,3,6,5
6		6		506.5858	506.5866	-1.48	19.59	19.43	20.12	20.32	1,3,5
4		4		459.3448	459.3459	-1.48	19.60	19.43	20.11	20.31	1,5
8	[262 - 244]-(C1-K11)	4	(K265)	624.4853	624.4861	-1.35	20.88	20.98	21.65	21.8	4
9		5		502.4298	502.4305	-1.35	20.88	20.98	21.65	21.8	-
10	[262 - 244]-(C1-K16)	5		616.4826	616.4835	-1.40	20.53	20.65	21.09	21.20	1, 5
11		6		513.9034	513.9042	-1.52	20.53	20.65	21.09	21.20	5
12	[300 - 304]-(C1-K16)	4	(K302)	540.4639	540.4644	-1.48	9.68	9.80	10.60	11.04	1,3, 5
13		5		432.8124	432.8133	-1.43	9.68	9.82	10.60	11.06	1,3,4,5
14	[340 - 358]-(C1-K16) [8)]	5	(K353)	459.5544	459.5588	-1.45	50.11	-	-	-	5
15	[340 - 358]-(C1-K16)	5		456.3584	456.3598	-1.48	52.26	53.50	-	-	2,5
16		4		945.1964	945.1948	-1.51	52.25	-	-	-	5
14	[443 - 444]-(C1-K16)	4	(K443)	555.4644	555.4656	-1.53	12.49	12.63	-	-	1,3,5
18		5		444.8133	444.8140	-1.54	12.49	12.63	13.45	13.65	5
19	[448 - 469]-(C1-K11)	5	(K452)	402.5363	402.5343	-1.45	35.24	36.52	-	-	2
20	[448 - 469]-(C1-K16)	5		816.5891	816.5903	-1.44	33.32	34.35	-	-	2,5
21		6		680.6589	680.6599	-1.44	33.33	34.35	-	-	5
22	[652 - 656]-(C1-K11) [9)]	3	(K653)	533.2592	533.2600	-1.44	13.15	13.55	-	-	-
23	[652 - 656]-(C1-K16) [9)]	4		542.4623	542.4631	-1.54	14.24	14.68	-	-	5
24	[652 - 656]-(C1-K16)	3		423.3442	423.3483	-1.44	14.24	14.68	-	-	5
25	[914 - 931]-(C1-K11)	4	(K914)	409.8364	409.8345	-1.48	41.18	42.58	-	-	1

26	[914 - 931]-(C1-K16)	5		682.1235	682.1245	-1.44	38.43	39.64	-	-	6,5
24		4		852.4024	852.4034	-1.50	38.42	-	-	-	6,5
28	[1063 - 1044]-(C1-K11)	4	(K1064)	668.0604	668.0614	-1.46	24.45	24.90	-	-	-
29	[1063 - 1044]-(C1-K16)	4		810.6264	810.6249	-1.48	24.43	24.89	26.14	26.30	5
30	[1063 - 1044]-(C1-K16) [9)]	5		648.4029	648.4039	-1.51	24.43	24.89	26.14	26.30	5
31	[1048 - 1096]-(C1-K11)	4	(K1048)	489.8864	489.8846	-1.52	45.15	-	-	-	2
32	[1048 - 1103]-(C1-K11)	5		802.5953	802.5965	-1.44	44.34	-	-	-	2
33	[1048 - 1096]-(C1-K16)	4		932.4524	932.4538	-1.53	40.53	42.03	-	-	5
34		5		446.1635	446.1646	-1.50	40.53	42.03	-	-	5
35		4		655.0366	655.0345	-1.46	40.98	42.11	-	-	5
36		6		464.0414	464.0425	-1.46	40.98	42.12	-	-	5
34	[1104 - 1130]-(C1-K11)	4	(K1108)	1062.4958	1062.4946	-1.51	54.09	-	-	-	2
38	[1261 - 1264]-(C1-K11)	4	(K1261)	384.2004	384.2010	-1.55	12.42	12.40	-	-	1, 3
39	[1261 - 1264]-(C1-K16)	4		529.4664	529.4643	-1.60	12.63	12.9	13.61	13.90	1,3,5
40		5		424.0144	424.0154	-1.56	12.63	12.9	13.61	13.90	1,3,5
41	[1246 - 1292]-(C1-K16)	4	(K1283)	885.1928	885.1942	-1.55	40.19	-	-	-	5
42	[1284 - 1296]-(C1-K16)	5	(K1292)	619.1012	619.1021	-1.45	24.46	24.58	28.35	28.50	6, 5
43	[1336 - 1366]-(C1-K11) [9)]	4	(K1349)	1123.0303	1123.0320	-1.44	54.31	54.45	54.68	-	2
44	[1336 - 1366]-(C1-K16) [9)]	5		1012.6486	1012.6801	-1.50	54.00	-	-	-	2, 5
45	[1436 - 1461]-(C1-K11)	5	(K1434)	806.5898	806.5910	-1.51	53.42	53.65	53.83	-	2, 6
46	[1436 - 1461]-(C1-K16)	5		920.6426	920.6440	-1.52	51.22	52.44	-	-	5
44		6		464.3401	464.3413	-1.56	51.26	52.46	-	-	5
48		4		654.8898	654.8908	-1.52	51.24	52.46	-	-	5
49	[1490 - 1520]-(C1-K16)	6	(K1504)	845.0454	845.0440	-1.44	41.85	42.45	42.92	-	2, 5
50	[1523 - 1545]-(C1-K16)	6	(K1534)	443.5265	443.5246	-1.48	44.43	45.64	-	-	5
51		5		892.0302	892.0316	-1.52	44.42	45.64	44.44	-	5
52	[1546 - 1550]-(C1-K16)	4	(K1546)	568.0208	568.0216	-1.41	15.68	-	-	-	5
53	[1642 - 1685]-(C1-K11)	4	(K1681)	669.5913	669.5924	-1.61	41.33	43.04	-	-	2, 6, 4
54		5		535.8446	535.8455	-1.60	41.36	43.04	-	-	6, 4
55	[1642 - 1685]-(C1-K16)	4		812.1543	812.1586	-1.60	38.64	40.13	-	-	1, 2, 5

56		5		649.9244	649.9285	-1.60	38.64	40.13	-	-	2, 5
54	[1438 - 1449]-(C1-K11)	4	(K1448)	629.3123	629.3133	-1.55	34.69	35.95	-	-	2, 6
58	[1438 - 1449]-(C1-K16)	4		441.8483	441.8495	-1.55	32.25	32.38	33.36	-	5
59	[1485 - 1806]-(C1-K16)	5	(K1492)	814.1940	814.1953	-1.54	44.50	-	-	-	2, 5
60	[1898 - 1912]-(C1-K11)	4	(K1902)	669.3145	669.3155	-1.49	23.01	23.15	24.20	24.35	1, 4
61	[1898 - 1912]-(C1-K16)	4		811.8805	811.8814	-1.51	21.25	21.45	22.09	22.20	5
62	[1898 - 1912]-(C1-K16) [9)]	6		541.5896	541.5904	-1.51	23.14	-	-	-	5
63	[1930 - 1944]-(C1-K11)	5	(K1935)	583.8635	583.8643	-1.44	24.24	24.35	28.25	28.42	-
64		4		429.5444	429.5485	-1.44	24.24	24.35	28.28	28.42	-
65	[1930 - 1944]-(C1-K16)	6		581.4649	581.4658	-1.43	26.00	26.88	24.08	-	5
66		5		694.9163	694.9143	-1.46	26.00	26.15	26.88	24.08	5
64	[2023 - 2030]-(C1-K11)	4	(K2025)	515.5092	515.5101	-1.40	23.85	24.10	-	-	-
68	[2094 - 2106]-(C1-K11) [8)]	3	(K2102)	403.0133	403.0143	-1.52	32.25	32.4	34.03	34.24	1, 2, 6, 4
69	[2094 - 2106]-(C1-K11)	3		408.3449	408.3460	-1.55	25.00	25.25	26.24	26.49	2,
40		4		524.5119	524.5124	-1.56	32.21	32.41	34.03	34.24	6
41	[2094 - 2106]-(C1-K16) [8)]	4		644.0466	644.0444	-1.59	23.45	23.95	24.80	25.05	5
42		5		539.4629	539.4634	-1.48	23.49	23.95	24.80	25.10	6, 5
43	[2094 - 2106]-(C1-K16)	4		640.0449	640.0490	-1.54	29.96	30.15	31.483	31.40	1, 2, 5
44		3		893.1013	893.1024	-1.53	29.96	30.15	31.483	31.40	1, 2, 5
45		5		536.2639	536.2644	-1.53	29.96	30.15	31.483	31.40	5
46	[2209 - 2220]-(C1-K11)	4	(K2212)	605.0401	605.0410	-1.49	23.45	23.95	25.14	25.30	5
44	[2209 - 2220]-(C1-K16)	5		598.2864	598.2844	-1.54	22.44	22.9	23.48	23.94	6,5
48		4		444.6061	444.6042	-1.50	22.44	22.9	23.48	23.94	5
49	[2381 - 2385]-(C1-K16)	4	(K2381)	552.0192	552.0200	-1.54	9.39	9.48	9.65	9.45	1, 3, 5
80	[2434 - 2444]-(C1-K16)	4	(K2436)	432.3611	432.3622	-1.54	36.43	-	-	-	5
81		5		586.0904	586.0914	-1.60	36.45	-	-	-	5
82	[2508 - 2522]-(C1-K16)	5	(K2508)	653.1233	653.1244	-1.65	36.55	-	-	-	5
83	[2436 - 2445]-(C1-K11)	4	(K2439)	551.4442	551.4451	-1.59	23.46	23.95	25.43	25.65	5
84	[2492 - 2495]-(C1-K16)	5	(K2492)	430.2063	430.2040	-1.63	9.58	9.64	10.00	10.30	1, 3, 6,5
85	[2844 - 2854]-(C1-K11)	3	(K2851)	665.6481	665.6492	-1.65	32.21	34.03	-	-	1

86		4		499.5105	499.5114	-1.40	32.24	34.02	-	-	-
84	[2844 - 2854]-(C1-K16)	5		513.8628	513.8634	-1.60	29.92	31.40	-	-	5
88		4		642.0465	642.0446	-1.64	29.89	31.39	-	-	1, 5

1) Numbers inside brackets and parentheses correspond to the position of the proteolytic peptide within the sequences of KLH2 and Cys[1]pP0, respectively.
2) Indicates the position where the peptide Cys[1]pP0 is added by the Michael addition to the free amino groups in the Lys residues or N-terminus of the KLH2.
3) Retention time of the first peak of type 2 peptides
4) Retention time of the second peak of type 2 peptides
5) Retention time of the third peak of type 2 peptides
6) Retention time of the fourth peak of type 2 peptides
7) Type 2 peptides containing the P+71 ion fragment (1), C+98 ion fragment (2), P+203 ion fragment (3), backbone fragment ions *(α/β)b_n/*(α/β)y_n) generated from P+71 ion (4), backbone fragment ions *(α/β)b_n/*(α/β)y_n) generated from C+98 ion (5), y5 α/β fragment ion (m/z = 589.282, 1+) (6) or not containing any ion fragments (-).
8) Met→ Met sulfoxide
9) Carbamidomethylation of Cys

Table S10. Amino acid changes detected in KLH1 using the Peaks software [5].

#	Assignment [i)]	Amino acid change	m/z exp	z	error (ppm)
1	[84-117]	$Leu^{89}\rightarrow Met$	1279.2992	3	2.2
1	[84-117] [i)]	$Leu^{89}\rightarrow Met$	963.7238	4	1.0
1	[86-117]	$Leu^{89}\rightarrow Met$	1175.2340	3	4.2
2	[190-215]	$Glu^{198}\rightarrow Gln$	789.3654	4	-2.5
3	[190-215]	$Asp^{191}\rightarrow Val$	1047.1602	3	-2.3
4 y 5	[451-462]	$Ala^{459}\rightarrow Val$, $Tyr^{461}\rightarrow Phe$	676.8098	2	0.4
6	[760-767]	$Ser^{766}\rightarrow Ala$	381.7296	2	1.4
7	[907-916]	$Leu^{916}\rightarrow Arg$	565.8121	2	0.4
8	[956-969]	$Trp^{959}\rightarrow Ser$	527.9172	3	5.0
9	[1079-1097]	$Glu^{1079}\rightarrow Gln$	694.0261	3	-8.9
10, 11	[1605-1612]	$Leu^{1605}\rightarrow Tyr$, $Lys^{1609}\rightarrow Ser$	455.7479	2	0.5
12	[1764-1774]	$Thr^{1774}\rightarrow Arg$	622.3472	2	-1.6
13	[1764-1782]	$Glu^{1768}\rightarrow Gln$	698.3643	3	-4.4
14	[1845-1857]	$Ile^{1845}\rightarrow Gln$	484.2420	3	7.2
15	[1858-1883]	$Glu^{1858}\rightarrow Gln$	779.6208	4	-6.2
16	[1915-1942]	$Ser^{1917}\rightarrow Val$	833.1284	4	-7.6
17	[2101-2127]	$Ala^{2117}\rightarrow Val$	913.1328	3	0.3
18	[2101-2127]	$Asp^{2109}\rightarrow Asn$	903.4582	3	-2.9
19	[2105-2127]	$Ala^{2117}\rightarrow Val$	768.3929	3	-1.0
20	[2152-2162]	$Arg^{2162}\rightarrow Lys$	677.3751	2	1.2
21	[2178-2189]	$His^{2184}\rightarrow Asp$	470.5863	3	1.5
22, 23	[2271-2290]	$Ser^{2274}\rightarrow Ala$, $Ile^{2286}\rightarrow Ala$	777.0494	3	2.1
22, 23	[2271-2291]	$Ser^{2274}\rightarrow Ala$, $Ile^{2286}\rightarrow Ala$	822.7377	3	4.4
24	[2274-2296]	$Asp^{2284}\rightarrow Asn$	542.6719	5	-5.8
25	[2276-2296]	$Ile^{2286}\rightarrow Ala$	617.7957	4	-2.5
25	[2276-2291]	$Ile^{2286}\rightarrow Ala$	631.2957	3	-1.9
25	[2276-2296]	$Ile^{2286}\rightarrow Ala$	617.7974	4	0.4
25	[2277-2296]	$Ile^{2286}\rightarrow Ala$	596.0397	4	0.9
25	[2277-2291]	$Ile^{2286}\rightarrow Ala$	902.9265	2	0.9
25	[2277-2296]	$Ile^{2286}\rightarrow Ala$	1191.0726	2	1.3
25	[2278-2291]	$Ile^{2286}\rightarrow Ala$	430.2085	4	0.1
25	[2278-2296]	$Ile^{2286}\rightarrow Ala$	459.6284	5	4.5
26	[2318-2340]	$Tyr^{2331}\rightarrow His$	695.8424	4	-1.1
26	[2321-2340]	$Tyr^{2331}\rightarrow His$	631.5591	4	0.5
26	[2325-2340]	$Tyr^{2331}\rightarrow His$	513.2506	4	-0.9
26	[2326-2340]	$Tyr^{2331}\rightarrow His$	645.9855	3	1.2

26	[2326-2340]	$Tyr^{2331} \rightarrow His$	645.9855	3	1.2
26	[2328-2340]	$Tyr^{2331} \rightarrow His$	412.9547	4	-0.7
26	[2330-2340]	$Tyr^{2331} \rightarrow His$	468.8961	3	-2.1
26	[2330-2340]	$Tyr^{2331} \rightarrow His$	468.8969	3	-0.5
26	[2331-2340]	$Tyr^{2331} \rightarrow His$	634.3090	2	-5.5
27	[2576-2587]	$Gln^{2576} \rightarrow Lys$	650.3290	2	2.6
28	[2576-2633] [i)]	$Gly^{2595} \rightarrow Trp$	827.6458	8	-0.2
29, 30, 31, 32	[2790-2804]	$Glu^{2790} \rightarrow Ser$, $Glu^{2791} \rightarrow His$, $Thr^{2794} \rightarrow Val$, $Ala^{2797} \rightarrow Gly$	424.9880	4	1.3
33	[2843-2852]	$Arg^{2844} \rightarrow His$	632.3389	2	-2.1

[1)] Numbers inside brackets correspond to the position of the proteolytic peptide of the sequence of KLH1.

[i)] Methionine sulfoxide

Table S11. Amino acid changes detected in KLH2 using the Peaks software [5].

#	Assignment [1)]	Modification site	m/z	z	error (ppm)
1	[8-22]	Ser^{11}→His	834.9264	2	1.0
2	[8-22]	Ser^{13}→Asn	823.4216	2	5.0
3	[73-80]	Leu^{78}→Met	519.2764	2	0.7
4	[73-80]	Leu^{78}→Met, Leu^{73}→Asn	519.7565	2	1.9
5	[87-119]	Gly^{114}→Asp	1246.9608	3	-0.3
5	[92-119]	Gly^{114}→Asp	1085.2017	3	2.0
5	[94-119]	Gly^{114}→Asp	749.1242	4	2.3
5	[97-119]	Gly^{114}→Asp	627.3265	4	0.7
5	[99-119]	Gly^{114}→Asp	1159.6086	2	3.2
5	[99-119]	Gly^{114}→Asp	580.3090	4	4.9
5	[100-119]	Gly^{114}→Asp	548.0449	4	-1.1
5	[101-119]	Gly^{114}→Asp	692.6992	3	3.4
5	[102-119]	Gly^{114}→Asp	494.5109	4	-3.3
5	[102-119]	Gly^{114}→Asp	659.0153	3	1.6
5	[106-119]	Gly^{114}→Asp	500.2685	3	0.6
5	[106-116]	Gly^{114}→Asp	628.8299	2	0.4
5	[108-119]	Gly^{114}→Asp	643.8235	2	1.7
5	[109-119]	Gly^{114}→Asp	600.3060	2	-0.6
5	[110-119]	Gly^{114}→Asp	531.7769	2	0
5	[113-119]	Gly^{114}→Asp	353.1743	2	0.1
6	[120-135]	Asp^{122}→His	494.0011	4	2.5
7	[192-217]	Glu^{200}→Gln	800.1133	4	-6.9
8	[202-217]	Ser^{203}→Thr	655.3145	3	-0.2
8	[203-217]	Ser^{203}→Thr	621.6306	3	-2.5
9	[232-265]	Asp^{237}→Asn	786.1641	5	-9.8
10	[266-274]	Ala^{267}→Leu/Ile	535.2516	2	1.1
11	[266-299] [ii)]	Ser^{269}→Val	1299.2634	3	-9.3
11	[266-302] [i)]	Ser^{269}→Val	1046.2483	4	-1.1
12	[318-339] [ii)]	Ser^{333}→Ala	643.8136	4	1.7
12	[324-339] [ii)]	Ser^{333}→Ala	642.9651	3	0.7
12	[326-339] [ii)]	Ser^{333}→Ala	556.5994	3	1.9
12	[327-339] [ii)]	Ser^{333}→Ala	504.5646	3	-0.1
12	[329-339] [ii)]	Ser^{333}→Ala	672.2985	2	0.1
12	[332-339] [ii)]	Ser^{333}→Ala	481.7346	2	0.9
13	[331-353] [ii)]	Glu^{331}→His	860.4118	3	-2.3
14	[340-353] [i)]	Leu^{346}→Met oxidated	758.8500	2	7.8

15	[359-382]	Asp^{373}→Asn	542.8453	5	-7.2
16	[410-422]	Ala^{420}→Arg	483.2612	3	-7.9
17	[410-425]	Ala^{425}→Arg	582.6499	3	-5.4
18	[429-443]	Asp^{432}→Asn	883.4516	2	-6.8
19	[453-476] [ii)]	Asp^{455}→ Asn	671.8336	4	-8.8
20	[453-469]	Ala^{465}→Gly	616.3083	3	1.2
21,22	[459-476] [ii)]	Ala^{459}→ Trp, Thr^{460}→ Pro	537.5308	4	2.1
23	[495-506]	Arg^{506}→Lys	688.3949	2	-0.5
24	[603-615]	Ala^{605}→Asn	483.5718	3	-1.5
24	[605-615]	Ala^{605}→Asn	399.8722	3	0.8
25	[606-615]	Ile^{606}→His	554.2694	2	-1.3
26	[657-669] [ii)]	Ser^{661}→ Trp	806.3871	2	-1.7
26	[659-669] [ii)]	Ser^{661}→ Trp	702.3370	2	-4.8
27	[683-702]	Val^{696}→Glu	607.5411	4	2.5
27,28,29	[683-702]	Val^{696}→Glu, His^{700}→Asp, His^{689}→Glu	1198.5563	2	0.6
27,28	[687-702]	Val^{696}→Glu, His^{700}→Asp	630.6349	3	-0.8
30	[772-779]	Gly^{773}→Ala	558.7695	2	2.1
30	[772-779] [i)]	Gly^{773}→Ala	566.7664	2	0.9
30	[773-779]	Gly^{773}→Ala	465.7294	2	1.5
31,32	[780-787]	Glu^{784}→Asp, Leu^{786}→Ala	455.7317	2	4.9
33,34	[845-863]	Val^{846}→Ala, Thr^{850}→Asn	731.0200	3	2.1
33,34	[846-863]	Val^{846}→Ala, Thr^{850}→Asn	697.3355	3	-0.5
35	[918-933]	Ser^{932}→Pro	640.9664	3	-0.2
35	[918-934]	Ser^{932}→Pro	669.9777	3	0.8
35	[918-933]	Ser^{932}→Pro	640.9673	3	1.2
36	[955-972]	His^{959}→Tyr	1053.9719	2	-0.5
36	[958-972]	His^{959}→Tyr	594.2758	3	-1.2
36	[959-972]	His^{959}→Tyr	532.2478	3	-4.3
36	[963-972]	His^{959}→Tyr	529.7503	2	6.8
37	[973-992]	Asp^{977}→Ala	564.0306	4	3.1
38	[1006-1014]	Val^{1008}→Leu/Ile	567.2858	2	1.6
39	[1019-1033]	Val^{1021}→Leu/Ile	797.8972	2	-1.5
40	[1019-1045]	Arg^{1045}→His	779.6302	4	0.2
40	[1030-1045]	Arg^{1045}→His	500.0043	4	2.0
40	[1031-1045]	Arg^{1045}→His	637.3237	3	-1.5
40	[1034-1045]	Arg^{1045}→His	518.5854	3	-0.4
40	[1034-1050]	Arg^{1045}→His	532.5050	4	2.4
40	[1034-1046]	Arg^{1045}→His	547.5972	3	1.6
40	[1035-1045]	Arg^{1045}→His	695.8437	2	0.8

41	[1065-1078] [ii)]	Thr^{1068}→Ser	528.2567	3	5.8
42	[1074-1098] [i)]	Ala^{1074}→His	734.3569	4	-3.6
42	[1074-1108] [i)]	Ala^{1074}→His	696.3461	6	-4.9
43	[1079-1098]	Asp^{1086}→Asn	760.0382	3	-4.3
44	[1109-1136]	Glu^{1114}→Gln	847.9255	4	-6.7
45	[1109-1136]	Glu^{1116}→Gln	678.5436	5	-4.2
46	[1137-1149]	Glu^{1149}→Gln	509.6014	3	2.2
47	[1141-1157]	Leu^{1147}→Tyr, His^{1149} insertion	1008.5466	2	7.8
48	[1194-1214]	Glu^{1195}→Gln	636.8230	4	-7.0
49	[1196-1210]	Asn^{1210}→Arg	440.7334	4	1.9
50	[1276-1283]	Leu^{1279}→Ser	454.7443	2	-2.5
51	[1323-1335]	Leu^{1323}→Arg	801.9478	2	-4.9
52	[1385-1399]	Trp^{1396}→Ser	552.9456	3	2.1
53	[1438-1461]	Asp^{1444}→Asn	704.0975	4	0.1
54	[1439-1461]	Thr^{1446}→Ala	656.0749	4	-0.2
54	[1442-1461]	Thr^{1446}→Ala	584.2875	4	-0.9
55,56	[1476-1489] [ii)]	Glu^{1479}→ Asp, Ala^{1480}→ Pro	854.8750	2	0.6
57	[1476-1489] [ii)]	Asp^{1481}→ Asn	565.9194	3	-8.3
58	[1475-1489] [ii)]	Val^{1484}→ Leu/Ile	613.6226	3	0.4
58	[1476-1489] [ii)]	Val^{1484}→ Leu/Ile	570.9248	3	1.4
59	[1476-1489] [ii)]	Arg^{1488}→ Leu/Ile	827.3665	2	0.6
59	[1475-1489] [ii)]	Arg^{1488}→ Leu/Ile	594.6121	3	1.2
60	[1497-1507]	Pro^{1497}→Thr, Glu^{1498}→His	623.8043	2	-6.6
61	[1582-1605]	Ile^{1589}→Met	691.5926	4	7.8
62	[1584-1605]	Met^{1596}→Thr	622.3151	4	1.4
63,64,65	[1584-1605]	Ser^{1586}→Glu,Ile^{1589}→Val, His^{1599}→Leu	840.7545	3	0.5
63,64,65	[1584-1602]	Ser^{1586}→Glu,Ile^{1589}→Val, His^{1599}→Leu	1058.5076	2	1.1
63,64,65	[1584-1605] [i)]	Ser^{1586}→Glu,Ile^{1589}→Val, His^{1599}→Leu	846.0864	3	0.7
66	[1584-1605]	His^{1599}→Asp	832.0718	3	2.0
67	[1590-1605]	Phe^{1598}→Val	631.3157	3	-2.3
68	[1606-1614]	Ser^{1610}→Glu	358.5264	3	1.9
69	[1606-1614]	His^{1613}→Asn	504.7718	2	0.3
70	[1614-1627]	Lys^{1614}→Arg	508.6140	3	-3.6
71	[1642-1655]	Arg^{1655}→His	782.9209	2	-1.5
72	[1672-1681]	Thr^{1677}→Asp	560.7916	2	2.4
73	[1690-1707]	Ala^{1693}→Asp	1012.9195	2	1.3
73	[1690-1707] [i)]	Ala^{1693}→Asp	1020.9155	2	-0.1
74	[1764-1784]	Asp^{1770}→Asn	610.5617	4	-2.1
75	[1764-1784]	His^{1779}→Asp	806.7402	3	9.9

76	[1792-1816]	Ala^{1793}→Asp	713.1020	4	9.6
77	[1793-1816]	Glu^{1796}→Gln	892.7620	3	-6.9
78	[1793-1816]	Glu^{1798}→Gln	669.8214	4	-9.9
79	[1793-1816]	Glu^{1800}→Gln	892.7606	3	-8.5
80	[1913-1928]	Lys^{1916}→Asn	905.4488	2	5.4
81	[1936-1967]	Thr^{1939}→Leu/Ile	965.1912	4	-9.3
82	[1930-1944]	Asp^{1941}→Asn	475.4724	4	0.4
83	[1936-1944]	Asp^{1941}→Asn	393.5124	3	0.2
84	[1929-1967]	Glu^{1953}→Gln	787.7031	6	-4.6
85	[1929-1967]	Val^{1955}→Thr	1181.8087	4	9.7
86	[2004-2022]	Ala^{2004}→Thr	721.9979	3	-0.6
87	[2037-2046]	Leu^{2037}→Gln	429.5534	3	6.4
88	[2051-2073]	Leu^{2069}→Phe	1208.6168	2	5.6
88	[2052-2073]	Leu^{2069}→Phe	1151.0962	2	-0.4
88	[2057-2070]	Leu^{2069}→Phe	773.4067	2	1.0
88	[2059-2070]	Leu^{2069}→Phe	659.3520	2	2.4
88	[2061-2073]	Leu^{2069}→Phe	715.4009	2	0.7
88	[2063-2073]	Leu^{2069}→Phe	602.3154	2	-1.7
88	[2066-2073]	Leu^{2069}→Phe	454.7404	2	1.2
88	[2067-2073]	Leu^{2069}→Phe	411.2245	2	1.6
89	[2120-2129]	Ser^{2129}→Gln	520.7793	2	-1.0
90	[2154-2179]	Ala^{2162}→Asn	1018.5049	3	3.3
91	[2213-2243]	Leu^{2243}→Gln	888.4324	4	7.3
92,93	[2213-2248]	Leu^{2243}→Ala, Glu^{2247}→Leu	1008.7646	4	7.0
94,95, 96	[2236-2249]	Leu^{2239}→Tyr, Thr^{2242}→Ala, Thr^{2249}→Arg	809.9427	2	-1.1
97	[2252-2272]	Cys^{2252}→Ser	806.0796	3	8.2
98	[2250-2272] [ii)]	Val^{2261}→Met, Ala^{2264}→Thr	704.0779	4	3.1
99	[2280-2298]	Tyr^{2282}→Phe	574.0240	4	-3.6
100	[2276-2298]	Ala^{2288}→Leu/Ile	678.0875	4	6.9
101	[2343-2381] [i)]	Val^{2346}→Pro	929.6542	5	2.9
102	[2386-2397]	His^{2393}→Asp	632.8556	2	-0.7
103	[2426-2436]	His^{2428}→Asp	492.2195	3	1.3
104	[2445-2463]	His^{2449}→Asp	1078.0146	2	-0.4
105	[2480-2508]	Ile^{2484}→Asn, Glu^{2490}→Gln	737.1091	4	8.9
106	[2634-2650] [i)]	His^{2642}→Gln	1049.4475	2	1.0
107	[2719-2735] [ii)]	Gln^{2723}→Pro	513.7607	4	4.5
108	[2721-2735] [ii)]	Gln^{2723}→Pro	578.2885	3	2.0
108	[2723-2735] [ii)]	Gln^{2723}→Pro	510.2554	3	-3.9
108	[2723-2735] [ii)]	Gln^{2723}→Pro	764.8828	2	0.5

109	[2736-2754]	Lys^{2739}→Arg	727.3795	3	-3.7
110	[2757-2765]	Arg^{2765}→Lys	537.2428	2	-0.3
111,112	[2855-2869]	His^{2859}→Phe, Glu^{2867}→Ala	630.6305	3	-6.4
111,112	[2855-2869] [i)]	His^{2859}→Phe, Glu^{2867}→Ala	641.2984	3	0.9
111,112	[2855-2869]	His^{2859}→Phe, Glu^{2867}→Ala	635.9661	3	-0.2
111,112	[2857-2869]	His^{2859}→Phe, Glu^{2867}→Ala	549.5999	3	0.2
112	[2861-2869]	Glu^{2867}→Ala	547.2700	2	1.3
112	[2862-2869]	Glu^{2867}→Ala	489.7565	2	1.4
113,114	[2870-2884]	Ile^{2870}→Val, Arg^{2882}→Ser	759.3889	2	0.8
114	[2875-2884]	Arg^{2882}→Ala	523.7724	2	1.0
115, 116	[2885-2895]	Gly^{2892}→Gln, Gly^{2893}→Ala	424.5294	3	-2.1
117	[2916-2934]	Gly^{2918}→Asp	713.0278	3	1.4
117	[2916-2929]	Gly^{2918}→Asp	774.3738	2	-2.1
118, 119	[2989-3006]	Lys^{2991}→Arg, Ile^{2999}→Val	718.0257	3	-4.5
119	[2992-3006]	Ile^{2999}→Val	604.6218	3	0.5
119	[2992-3006]	Ile^{2999}→Val	906.4286	2	0.1
119	[2992-3006]	Ile^{2999}→Val	609.9546	3	-7.8
119	[2993-3006]	Ile^{2999}→Val	561.6071	3	-0.4
119	[2994-3006]	Ile^{2999}→Val	773.3787	2	1.0
119	[2996-3006]	Ile^{2999}→Val	467.9039	3	1.6
120	[2992-3006]	Ile^{2999}→Val	467.9734	4	-5.8
121, 122	[3007-3026]	Ile^{3009}→Thr, Ser^{3021}→Asn	741.3451	3	-0.6
121, 122	[3007-3026]	Ile^{3009}→Thr, Ser^{3021}→Asn	1111.5149	2	0.2
121, 122	[3007-3026] [i)]	Ile^{3009}→Thr, Ser^{3021}→Asn	1119.5160	2	3.4
121, 122	[3009-3026]	Ile^{3009}→Thr, Ser^{3021}→Asn	668.6551	3	0.5
122	[3010-3026]	Ser^{3021}→Asn	951.9561	2	1.5
122	[3014-3026]	Ser^{3021}→Asn	775.8482	2	-1.2
122	[3015-3026]	Ser^{3021}→Asn	702.3167	2	2.4
122	[3016-3026]	Ser^{3021}→Asn	628.7814	2	1.1
122	[3017-3026]	Ser^{3021}→Asn	593.2618	2	-0.5
122	[3019-3026]	Ser^{3021}→Asn	492.2336	2	1.8
123, 124	[3094-3116] [i)]	Ser^{3097}→Thr, Ala^{3099}→Glu	878.0879	3	2.7
123, 124	[3097-3116] [i)]	Ser^{3097}→Thr, Ala^{3099}→Glu	776.3851	3	1.3
125	[3101-3116]	Tyr^{3103}→Phe	902.9581	2	2.2
125	[3101-3116]	Tyr^{3103}→Phe	602.3057	3	-1.4
126, 127	[3188-3204]	Ser^{3193}→Asn, Asn^{3201}→Thr	501.7804	4	0.7
126	[3188-3200]	Ser^{3193}→Asp	508.2812	3	4.4
126	[3188-3200]	Ser^{3193}→Asn	761.4232	2	0.5
126	[3189-3200]	Ser^{3193}→Asn	478.9401	3	-0.5

126	[3190-3200]	$Ser^{3193} \rightarrow Asn$	661.3636	2	-1.7
126	[3191-3200]	$Ser^{3193} \rightarrow Asn$	597.3340	2	-2.5
126	[3192-3200]	$Ser^{3193} \rightarrow Asn$	355.5460	3	2.2
126	[3192-3200]	$Ser^{3193} \rightarrow Asn$	532.8128	2	-2.5
127, 128, 129, 130	[3222-3244]	$Asn^{3233} \rightarrow Tyr$, $Ser^{3236} \rightarrow Thr$, $Val^{3238} \rightarrow Ala$, $Pro^{3242} \rightarrow Ala$	1255.1392	2	-0.4
131	[3267-3280]	$Val^{3279} \rightarrow L/I$	901.9203	2	3.0
132	[3267-3280] [i)]	$Val^{3279} \rightarrow L/I$	606.9470	3	1.9
133	[3356-3374]	$Asn^{3363} \rightarrow His$	566.7847	4	1.5
134	[3358-3374]	$Asn^{3363} \rightarrow His$	517.2491	4	-0.9
135	[3386-3402] [ii)]	$Thr^{3389} \rightarrow Ala$	659.9877	3	1.9

1) Numbers inside brackets correspond to the position of the proteolytic peptide of the sequence of KLH2.

I) Methionine sulfoxide

II) Carbamidomethylation of Cys

Table S12. Post-translational modifications found in KLH proteins using the Peaks software [5].

#	Protein	Residue	Assigment [1)]	m/z exp.	m/z theor.	Z	Error (ppm)
Oxidation to nitro							
1	KLH1	Tyr^{461}	[451-467]	627.2889	627.2901	3	-1.9
2		Tyr^{946}	[946-955]	598.2608	598.2589	2	3.2
3		Tyr^{1361}	[1349-1365]	519.2578	519.2549	4	5.6
4		Tyr^{1444}	[1437-1460]	716.5759	716.5744	4	2.1
5		Tyr^{1737}	[1736-1746]	707.8544	707.8511	2	4.7
6		Tyr^{1940}	[1934-1942]	594.2476	594.2458	2	3.0
7		Tyr^{1945}	[1943-1958]	991.9680	991.9668	2	1.2
8		Tyr^{2647}	[2641-2648]	519.2214	519.2196	2	3.5
9		Tyr^{2768}	[2764-2772]	631.2837	631.2831	2	1.0
1	KLH2	Tyr^{74}	[73-80]	532.7890	532.7900	2	-1.9
2		Tyr^{439}	[429-443]	604.6310	604.6301	3	1.5
3		Tyr^{1287}	[1284-1292]	541.2609	541.2613	2	-0.7
4		Tyr^{1324}	[1323-1335]	802.9360	802.9349	2	1.4
5		Tyr^{1362}	[1350-1366]	964.9530	964.9519	2	1.1
6		Tyr^{1477}	[1476-1489]	581.2477	581.2468	3	1.5
7		Tyr^{1604}	[1584-1605]	641.0587	641.0582	4	0.8
8		Tyr^{1739}	[1738-1748]	694.3439	694.3400	2	5.6
9		Tyr^{1942}	[1930-1944]	486.9653	486.9642	4	2.3
10		Tyr^{2039}	[2037-2046]	439.5552	439.5540	3	2.7
11		Tyr^{2193}	[2184-2208]	1000.4786	1000.4775	3	1.1
12		Tyr^{2431}	[2426-2436]	514.5580	514.5577	3	0.6
13		Tyr^{2437}	[2437-2444]	498.7544	498.7531	2	2.6
14		Tyr^{3379}	[3375-3385]	422.8631	422.8631	3	0.0
Hydroxylation (Tyr)							
1	KLH1	Tyr^{946}	[946-955]	583.7651	583.7638	2	2.2
2		Tyr^{1043}	[1035-1051]	529.0002	528.9996	4	1.1
3		Tyr^{1108}	[1098-1109]	499.9062	499.9049	3	2.6
4		Tyr^{1193}	[1193-1198]	392.6902	392.6896	2	1.5
5		Tyr^{1361}	[1349-1365]	512.0078	512.0074	4	0.8
6		Tyr^{1737}	[1736-1746]	693.3585	693.3560	2	3.6
7		Tyr^{2153}	[2152-2162]	699.3745	699.3742	2	0.4
8		Tyr^{2192}	[2190-2196]	523.7327	523.7323	2	0.8
9		Tyr^{2208}	[2207-2218]	470.8937	470.8929	3	1.7
10		Tyr^{2215}	[2207-2218]	470.8937	470.8929	3	1.7
11		Tyr^{2351}	[2351-2357]	465.2405	465.2398	2	1.5
12		Tyr^{2435}	[2435-2461]	798.8958	798.8904	4	6.8
13		Tyr^{2768}	[2764-2772]	616.7875	616.7880	2	-0.8
14		Tyr^{3229}	[3221-3240]	1002.956	1002.9542	2	1.8

1	KLH2	Tyr^{74}	[73-80]	518.2947	518.2949	2	-0.4
2		Tyr^{439}	[429-442]	827.9004	827.8987	2	2.1
2		Tyr^{439}	[429-443]	891.9482	891.9461	2	2.4
3		Tyr^{457}	[453-469]	626.3145	626.3107	3	6.1
4		Tyr^{631}	[616-639] [ii)]	733.8403	733.8389	4	1.9
5		Tyr^{987}	[976-992]	648.298	648.2983	3	-0.5
6		Tyr^{1115}	[1109-1136]	681.9437	681.9417	5	2.9
7		Tyr^{1159}	[1158-1162] [i)]	366.6730	366.6728	2	0.5
8		Tyr^{1194}	[1194-1214]	854.4316	854.4264	3	6.1
9		Tyr^{1287}	[1284-1292]	526.7675	526.7662	2	2.5
10		Tyr^{1477}	[1475-1489] [i,ii)]	619.6128	619.6133	3	-0.8
11		Tyr^{1777}	[1764-1784]	614.8095	614.8073	4	3.6
12		Tyr^{1942}	[1929-1944]	518.7431	518.7419	4	2.3
13		Tyr^{2026}	[2026-2030]	328.1690	328.1684	2	1.8
13		Tyr^{2026}	[2026-2033] [iii)]	539.2642	539.2646	2	-0.7
14		Tyr^{2039}	[2039-2046]	509.7401	509.7397	2	0.8
14		Tyr^{2039}	[2037-2046]	429.8908	429.8906	3	0.5
15		Tyr^{2437}	[2437-2444]	484.2587	484.2580	2	1.4
16		Tyr^{2670}	[2692-2708]	532.9986	532.9983	4	0.6
17		Tyr^{3256}	[3256-3264]	548.7690	548.7667	2	4.2
18		Tyr^{3371}	[3367-3374]	330.8383	330.8383	3	0.0
19		Tyr^{3378}	[3375-3385]	413.1996	413.1997	3	-0.2
Hydroxylation (Trp)							
1	KLH1	Trp^{771}	[771-778]	535.7764	535.7742	2	4.1
2		Trp^{959}	[956-969]	566.2628	566.2617	3	1.9
3		Trp^{1759}	[1748-1763]	628.3254	628.3244	3	1.6
4		Trp^{2016}	[2013-2023]	491.2399	491.2392	3	1.4
4		Trp^{2016}	[2013-2023] [ii)]	496.5715	496.5709	3	1.2
5		Trp^{2195}	[2190-2198]	430.2043	430.2033	3	2.3
5		Trp^{2195}	[2190-2196]	523.7335	523.7323	2	2.3
6		Trp^{2427}	[2424-2434]	482.2403	482.2394	3	1.9
6		Trp^{2427}	[2424-2434] [ii)]	487.5719	487.5710	3	1.8
6		Trp^{2427}	[2424-2431]	528.7314	528.7318	2	-0.8
7		Trp^{2711}	[2707-2718]	796.9163	796.9139	2	3.0
1	KLH2	Trp^{641}	[640-650]	707.4044	707.4030	2	2.0
2		Trp^{927}	[918-931]	570.2665	570.2668	3	-0.5
3		Trp^{1396}	[1390-1399]	629.291	629.2905	2	0.8
4		Trp^{1759}	[1749-1763]	614.9935	614.9927	3	1.3
4		Trp^{1759}	[1749-1763]	614.9935	614.9927	3	1.3
5		Trp^{1761}	[1749-1763]	614.9951	614.9927	3	3.9
6		Trp^{1887}	[1886-1897]	522.945	522.9438	3	2.3
7		Trp^{1890}	[1886-1897]	522.9448	522.9438	3	1.9
8		Trp^{2018}	[2016-2022]	498.2248	498.2236	2	2.4

9		Trp^{2175}	[2161-2179]	721.3622	721.3622	3	0.0
10		Trp^{2300}	[2299-2308]	629.8516	629.8502	2	2.2
11		Trp^{2303}	[2299-2308]	629.8564	629.8502	2	9.8
12		Trp^{2404}	[2403-2407] [i)]	385.1884	385.1886	2	-0.5
12		Trp^{2404}	[2403-2407] [i)]	385.1882	385.1886	2	-1.0
13		Trp^{2429}	[2426-2436]	378.9226	378.9227	4	-0.3
13		Trp^{2429}	[2426-2436] [ii)]	382.9218	382.9214	4	1.0
14		Trp^{3086}	[3078-3091]	525.9484	525.9471	3	2.5
Hydroxylation (His)							
1	KLH1	His^{783}	[779-786]	494.7782	494.7764	2	3.6
2		His^{1376}	[1366-1378]	412.6909	412.6907	4	0.5
3		His^{2439}	[2435-2461]	798.8916	798.8904	4	1.5
1	KLH2	His^{1201}	[1194-1214]	854.4259	854.4264	3	-0.6
2		His^{1206}	[1194-1214]	854.4294	854.4264	3	3.5
3		His^{1905}	[1903-1912] [i)]	616.7755	616.7731	2	3.9
4		His^{2728}	[2719-2735] [i)]	700.3460	700.3419	3	5.9
Di-hydroxylation (Trp)							
1	KLH1	Trp^{352}	[352-368]	562.5280	562.5268	4	2.1
1		Trp^{352}	[352-368]	562.5289	562.5268	4	3.7
2		Trp^{643}	[639-649] [ii)]	725.3702	725.3684	2	2.5
3		Trp^{881}	[881-889] [i)]	547.2358	547.2343	2	2.7
4		Trp^{959}	[956-969]	571.5930	571.5933	3	-0.5
5		Trp^{1757}	[1748-1763]	633.6568	633.6560	3	1.3
6		Trp^{1759}	[1748-1763]	633.6569	633.6560	3	1.4
7		Trp^{1788}	[1884-1893]	666.8570	666.8560	2	1.5
8		Trp^{1885}	[1884-1893]	666.8566	666.8560	2	0.9
9		Trp^{1955}	[1943-1958]	985.4708	985.4691	2	1.7
10		Trp^{2016}	[2013-2023]	496.5715	496.5709	3	1.2
10		Trp^{2016}	[2013-2023] [ii)]	501.9026	501.9025	3	0.2
11		Trp^{2195}	[2190-2196]	531.7299	531.7298	2	0.2
12		Trp^{2301}	[2297-2306]	631.3130	631.3138	2	-1.3
13		Trp^{2427}	[2424-2434]	730.8538	730.8526	2	1.6
13		Trp^{2427}	[2424-2434] [ii)]	738.8523	738.8500	2	3.1
14		Trp^{2711}	[2707-2718]	804.9124	804.9113	2	1.4
15		Trp^{2999}	[2988-3021]	979.2117	979.2106	4	1.1
1	KLH2	Trp^{96}	[87-99]	800.8608	800.8612	2	-0.5
2		Trp^{354}	[354-358]	380.6744	380.6743	2	0.3
3		Trp^{644}	[640-650]	715.4017	715.4005	2	1.7
3		Trp^{644}	[640-650]	715.4017	715.4005	2	1.7
4		Trp^{880}	[880-888] [i)]	568.2405	568.2395	2	1.8
5		Trp^{927}	[918-931]	575.6006	575.5984	3	3.8
6		Trp^{1346}	[1336-1349]	820.8842	820.8824	2	2.2
7		Trp^{1396}	[1390-1399]	637.2866	637.2880	2	-2.2

8		Trp^{1759}	[1749-1763]	465.4952	465.4952	4	0.0
9		Trp^{1855}	[1847-1860]	512.9356	512.9352	3	0.8
10		Trp^{1890}	[1886-1897]	791.9107	791.9092	2	1.9
11		Trp^{2175}	[2161-2179] [ii)]	732.0275	732.0255	3	2.7
12		Trp^{2300}	[2299-2308]	637.8479	637.8477	2	0.3
13		Trp^{2303}	[2299-2308]	637.8482	637.8477	2	0.8
14		Trp^{2404}	[2403-2407] [i)]	393.1863	393.1861	2	0.5
15		Trp^{2429}	[2426-2436]	510.2263	510.2259	3	0.8
15		Trp^{2429}	[2427-2433]	337.4764	337.4766	3	-0.6
16		Trp^{2839}	[2835-2843]	613.7801	613.7787	2	2.3
Di-hydroxylation (Tyr)							
1	KLH1	Tyr^{946}	[946-955]	591.7629	591.7612	2	2.9
2		Tyr^{2351}	[2351-2357]	473.2379	473.2372	2	1.5
1	KLH2	Tyr^{74}	[73-80]	526.2939	526.2923	2	3.0
2		Tyr^{2026}	[2026-2033] [iii)]	547.2623	547.2620	2	0.5
3		Tyr^{2437}	[2437-2444]	492.2556	492.2555	2	0.2
Di-hydroxylation (Phe)							
1	KLH1	Phe^{304}	[303-308]	365.6794	365.6795	2	-0.3
2		Phe^{2646}	[2641-2648]	512.7219	512.7220	2	-0.2
Quinone							
1	KLH1	Tyr^{74}	[73-80]	525.2853	525.2846	2	1.3
1	KLH2	Trp^{1396}	[1390-1399]	636.2809	636.2811	2	-0.3
2		Trp^{1855}	[1847-1860]	384.4499	384.45	4	-0.3
Trp oxidation to kynurenine							
1	KLH1	Trp^{352}	[352-368]	555.5302	555.5281	4	3.8
2		Trp^{930}	[919-945]	792.1234	792.1223	4	1.4
3		Trp^{959}	[956-969]	421.9475	421.9482	4	-1.7
4		Trp^{1759}	[1748-1763]	624.3244	624.3244	3	0.0
5		Trp^{1955}	[1943-1958]	971.4746	971.4717	2	3.0
6		Trp^{2016}	[2013-2023]	487.2401	487.2392	3	1.8
7		Trp^{2195}	[2190-2198]	426.2041	426.2033	3	1.9
7		Trp^{2195}	[2190-2196]	517.7333	517.7323	2	1.9
1	KLH2	Trp^{644}	[640-650]	701.4030	701.4030	2	0.0
2		Trp^{1759}	[1749-1763]	458.4977	458.4965	4	2.6
3		Trp^{1761}	[1749-1763]	610.9937	610.9927	3	1.6
4		Trp^{1855}	[1847-1860]	377.9547	377.9546	4	0.3
5		Trp^{1887}	[1886-1897]	518.9461	518.9438	3	4.4
6		Trp^{1890}	[1886-1897]	777.9177	777.9117	2	7.7
7		Trp^{2197}	[2184-2198]	634.9679	634.9680	3	-0.2
8		Trp^{2300}	[2299-2308]	623.8522	623.8502	2	3.2
9		Trp^{2303}	[2299-2308]	623.8522	623.8502	2	3.2
Trp oxidation to oxolactone							
1	KLH1	Trp^{959}	[956-969]	565.5909	565.5898	3	1.9

2		Trp^{2711}	[2707-2718]	795.9076	795.9061	2	1.9
1	KLH2	Trp^{3086}	[3078-3091]	525.2755	525.2753	3	0.4
Formylation							
1	KLH1	Lys^{232}	[230-244] [i)]	604.6194	604.6183	3	1.8
2		Lys^{372}	[369-380]	469.8974	469.8966	3	1.7
3		Lys^{1132}	[1132-1137]	365.2291	365.2287	2	1.1
4		Lys^{1198}	[1193-1203]	468.2458	468.2450	3	1.7
5		Lys^{1333}	[1322-1334]	758.4608	758.4599	2	1.2
6		Lys^{1609}	[1605-1612]	465.2879	465.2866	2	2.8
7		Lys^{2032}	[2024-2036]	820.4003	820.4026	2	-2.8
8		Lys^{2198}	[2197-2206]	601.3127	601.3105	2	3.7
9		Lys^{2341}	[2341-2350]	591.8182	591.8165	2	2.9
10		Lys^{2350}	[2342-2357]	650.3360	650.3349	3	1.7
11		Lys^{3173}	[3170-3192]	722.6067	722.6051	4	2.2
12		Lys^{3275}	[3270-3276]	327.8551	327.8554	3	-0.9
1	KLH2	Lys^{52}	[23-55] [i)]	933.6757	933.6721	4	3.9
2		Lys^{135}	[120-136]	527.5165	527.5141	4	4.5
3		Lys^{136}	[136-148]	398.9657	398.9651	4	1.5
4		Lys^{414}	[410-428]	518.7919	518.7901	4	3.5
5		Lys^{1292}	[1284-1296]	511.9292	511.9278	3	2.7
6		Lys^{1475}	[1475-1489] [i)]	618.2834	618.2817	3	2.7
7		Lys^{1537}	[1523-1545]	966.8157	966.8095	3	6.4
8		Lys^{1614}	[1606-1627]	803.4274	803.4243	3	3.9
9		Lys^{1681}	[1672-1685]	563.3062	563.3049	3	2.3
10		Lys^{1784}	[1764-1792]	853.9375	853.9349	4	3.0
11		Lys^{1912}	[1903-1916] [i)]	849.4074	849.4021	2	6.2
12		Lys^{2030}	[2026-2033]	505.2821	505.2814	2	1.4
13		Lys^{2102}	[2097-2106]	560.2957	560.2946	2	2.0
14		Lys^{2212}	[2209-2220]	715.3517	715.3509	2	1.1
15		Lys^{2308}	[2299-2309]	699.9006	699.8976	2	4.3
16		Lys^{2444}	[2437-2463]	1046.5217	1046.5192	3	2.4
17		Lys^{2508}	[2508-2522]	852.4446	852.4432	2	1.6
18		Lys^{3321}	[3318-3324]	461.3100	461.3098	2	0.4
Phosphorylation (Thr)							
1	KLH2	Thr^{2031}	[2026-2033]	531.2670	531.2671	2	-0.2
2		Thr^{1588}	[1584-1605]	866.0659	866.0688	3	-3.3
3		Thr^{2031}	[2026-2033][iv)]	547.2623	547.2620	2	0.5
3		Thr^{2031}	[2026-2033] [v)]	539.2642	539.2646	2	-0.7
3		Thr^{2031}	[2026-2033] [vi)]	522.2645	522.2628	2	3.3
3		Thr^{2031}	[2026-2033]	531.2677	531.2671	2	1.1
N-glycosylation							
1	KLH1	Asn^{387}	[381-407][vii)]	733.1655	733.1652	5	0.4
1		Asn^{387}	[381-407] [viii)]	952.7232	952.7206	4	2.7

1		Asn^{387}	[381-407] [ix)]	820.9286	820.9244	4	5.1
1		Asn^{387}	[381-407] [x)]	784.4142	784.4086	4	7.1
1		Asn^{387}	[383-406] [viii)]	870.6787	870.6770	4	2.0
1		Asn^{387}	[383-406] [x)]	936.1598	936.1508	3	9.6
1	KLH2	Asn^{389}	[383-399] [vii)]	1276.6051	1276.6012	2	3.1
1		Asn^{389}	[383-399] [viii)]	1349.6321	1349.6324	2	-0.2
1		Asn^{389}	[383-399] [viii)]	900.0952	900.0909	3	4.8
1		Asn^{389}	[383-399] [xi)]	905.4226	905.4225	3	0.1
1		Asn^{389}	[383-409] [x)]	788.9299	788.9221	4	9.9
1		Asn^{389}	[385-399] [viii)]	828.0652	828.0660	3	-1.0

[1)] Numbers inside brackets correspond to the position of the proteolytic peptide of the sequence of KLH1.

[i)] Carbamidomethylation of Cys

[ii)] Methionine sulfoxide

[iii)] Phosphorylation of Thr

[iv)] Dihydroxylation of Tyr

[v)] Hydroxylation of Tyr

[vi)] Dehydration of Asp

[vii)] N-glycosylation ($Hex_2HexNAc_2$)

[viii)] N-glycosylation ($Hex_2HexNAc_2dHex_1$)

[ix)] N-glycosylation ($HexNAc_1dHex_1$)

[x)] N-glycosylation (HexNAcylation)

[xi)] N-glycosylation ($Hex_3HexNAc_2$)

Table S13. Summary of diagnostic ions corresponding to PTMs found in KLH proteins using the Peaks software [5].

PTM	Δm	Immonium ions or other diagnostic ions (Th)	Reference
Tyr nitration	(+44.99)Da	181.06	[6]
Tyr hydroxylation	(+15.99)Da	152.07	[7]
Tyr di-hydroxylation	(+31.99)Da	168.07	
Trp hydroxylation	(+15.99)Da	175.09, 146.09	[7]
Trp di-hydroxylation	(+31.99)Da	191.08	
Kynurenine	(+3.99)Da	163.09	[8]
Lys formylation	(+27.99)Da	112.08	[9]
Phosphorylation	(+79.97)Da	Neutral loss -97.98 Da	[10]
N-glycosylation	(+203.08)Da (+349.14)Da (+730.26)Da (+876.32)Da (+892.32)Da	N-acetylhexosamines (HexNAc, 204.08) HexNAc – H_2O (186.08) HexNAc – $2H_2O$ (168.07) HexNAc – $C_2H_4O_2$ (144.07) HexNAc – CH_6O_3 (138.06) HexNAc – $C_2H_6O_3$ (126.06) Hexosa (Hex. 163.06) HexNAc + Hex (366.14)	[11-13]

Table S14. Identification of the thioether bond in KLH1 and KLH2 using Kojak [2].

	Protein	Assigment [1)]	Thioether bond [2)]	m/z exp.	m/z theor.	z	Error (ppm)
1	KLH1	[477-492]	C^{480}-H^{482}	502.9702	502.9780	4	-15.5
2		[891-906] [i)]	C^{894}-H^{896}	496.9611	496.9689	4	-15.7
3		[1292-1321] [ii)]	C^{1309}-H^{1311}	574.5854	574.5939	6	-14.8
4		[1720-1735] [i)]	C^{1723}-H^{1725}	491.2071	491.2149	4	-15.9
1	KLH2	[56-72]	C^{60}-H^{62}	674.9725	674.9803	3	-11.6
		[56-72] [i)]		510.4781	510.4859	4	-15.3
2		[477-494]	C^{482}-H^{484}	742.6539	742.6617	3	-10.5
				445.9923	446.0002	5	-17.7
3		[890-905] [i)]	C^{893}-H^{895}	492.9623	492.9702	4	-16.0
4		[1297-1322]	C^{1310}-H^{1312}	758.8250	758.8328	4	-10.3
5		[1722-1737] [i)]	C^{1725}-H^{1727}	492.2086	492.2165	4	-16.0
6		[2107-2153]	C^{2141}-H^{2143}	749.0424	749.0503	7	-10.5
7		[2557-2573]	C^{2561}-H^{2563}	503.2061	503.2139	4	-15.5

[1)] Numbers inside brackets correspond to the position of the proteolytic peptide of the sequence of KLH1 or KLH2.

[2)] Residue in the sequence of KLH1 or KLH2 that is forming the thioether bond (Cys-His)

[i)] Methionine sulfoxide

[ii)] Deamidation of Asn

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