

1 Table S1. MS/MS data of OA-NO₂ modified peptide 122-154. List of theoretical *m/z* values of fragment
 2 ions from peptide GASEGWC₁₂₈PYC₁₃₁GSPYSFLPQLNPGDIVAGQYEVK and its corresponding ion
 3 +200Da. y- and b-ions detected by MALDI MS are highlighted in bold. The observed mass shift after OA-
 4 NO₂ treatment was 198/200 Da.
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#	b	b + 200	Residue	y	y + 200	#
1	58,03	258,03	G			33
2	129,07	329,07	A	3475,60	3675,60	32
3	216,10	416,10	S	3404,56	3604,56	31
4	345,14	545,14	E	3317,53	3517,53	30
5	402,16	602,16	G	3188,49	3388,49	29
6	588,24	788,24	W	3131,47	3331,47	28
7	690,24	890,24	C	2945,39	3145,39	27
8	787,30	987,30	P	2842,38	3042,38	26
9	950,36	1150,36	Y	2745,32	2945,32	25
10	1052,36	1252,36	C	2582,26	2782,26	24
11	1109,38	1309,38	G	2479,25	2679,25	23
12	1196,41	1396,41	S	2422,23	2622,23	22
13	1293,47	1493,47	P	2335,20	2535,20	21
14	1456,53	1656,53	Y	2238,15	2438,15	20
15	1543,56	1743,56	S	2075,08	2275,08	19
16	1690,63	1890,63	F	1988,05	2188,05	18
17	1803,72	2003,72	L	1840,98	2040,98	17
18	1900,77	2100,77	P	1727,90	1927,90	16
19	2028,83	2228,83	Q	1630,84	1830,84	15
20	2141,91	2341,91	L	1502,79	1702,79	14
21	2255,95	2455,95	N	1389,70	1589,70	13
22	2353,01	2553,01	P	1275,66	1475,66	12
23	2410,03	2610,03	G	1178,61	1378,61	11
24	2525,05	2725,05	D	1121,58	1321,58	10
25	2638,14	2838,14	I	1006,56	1206,56	9
26	2737,21	2937,21	V	893,47	1093,47	8
27	2808,24	3008,24	A	794,41	994,41	7
28	2865,27	3065,27	G	723,37	923,37	6
29	2993,32	3193,32	Q	666,35	866,35	5
30	3156,39	3356,39	Y	538,29	738,29	4
31	3285,43	3485,43	E	375,22	575,22	3
32	3384,50	3584,50	V	246,18	446,18	2
33	3512,59	3712,59	K	147,11	347,11	1

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Table S1

1 Table S2. **Identification of modified residues within PknG Δ 74/TPR sequence.**

Peptide from-to	Modified residue	Assigned sequence ^a
Peptides containing modified cysteine residues ($\Delta m=198/200/202$ Da)		
105 - 111	C ₁₀₆ or C ₁₀₉	FCWNCGR
105 - 115	C ₁₀₆ or C ₁₀₉	FCWNCGRPVGR
122 - 144	C ₁₂₈ or C ₁₃₁	GASEGWCPYCGSPYSFLPQLNPGDIVAGQYEVK
Peptides containing modified histidine residues ($\Delta m=327$ Da)		
182 - 199	H ₁₈₅	GLVHSGDAEAQAMAMAER
200 - 222	H ₂₀₇ or H ₂₁₉	QFLAEVVHPSIVQIFNFVEHTDR

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3 ^aThe sequences and nitroalkylation sites were confirmed by MS/MS analysis.
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Table S2