

# Supporting Information

## Specific detection of protein carbonylation sites by 473 nm photo-dissociation mass spectrometry

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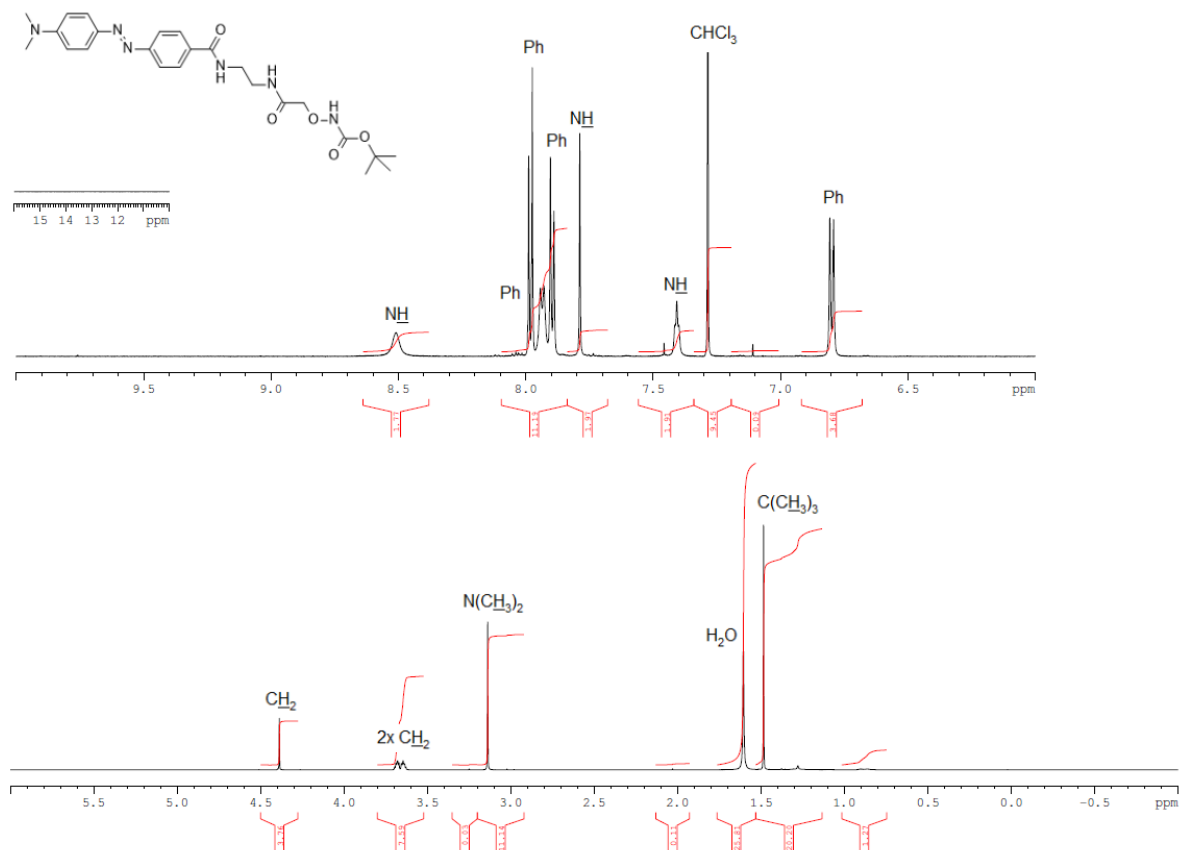


Figure S1 – <sup>1</sup>H NMR spectrum of the synthesized Dabcyl-Aoo-Boc

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ/ppm 8.51(bs, 1H), 7.97-8.00 (m, 2H), 7.94 (d, J=8.2 Hz, 2H), 7.88-7.91 (m, 2H), 7.79 (s, 1H), 7.41 (t, J=4.8 Hz, 1H), 6.80 (d, J=9.0 Hz, 2H), 4.39 (s, 2H), 3.66-3.70 (m, 2H), 3.62-3.66 (m, 2H), 3.14 (s, 6H), 1.49 (s, 9H).

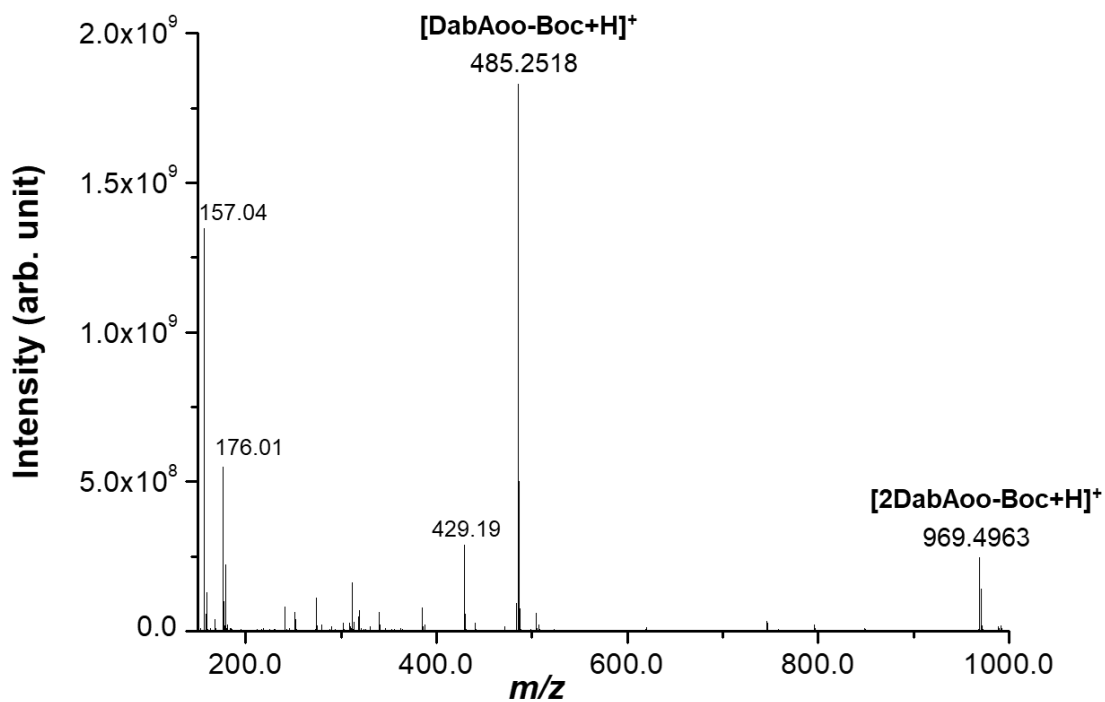


Figure S2 – Positive MS spectrum of the DabAoo-boc chromophore. Other peaks correspond to interfering synthesis intermediates.

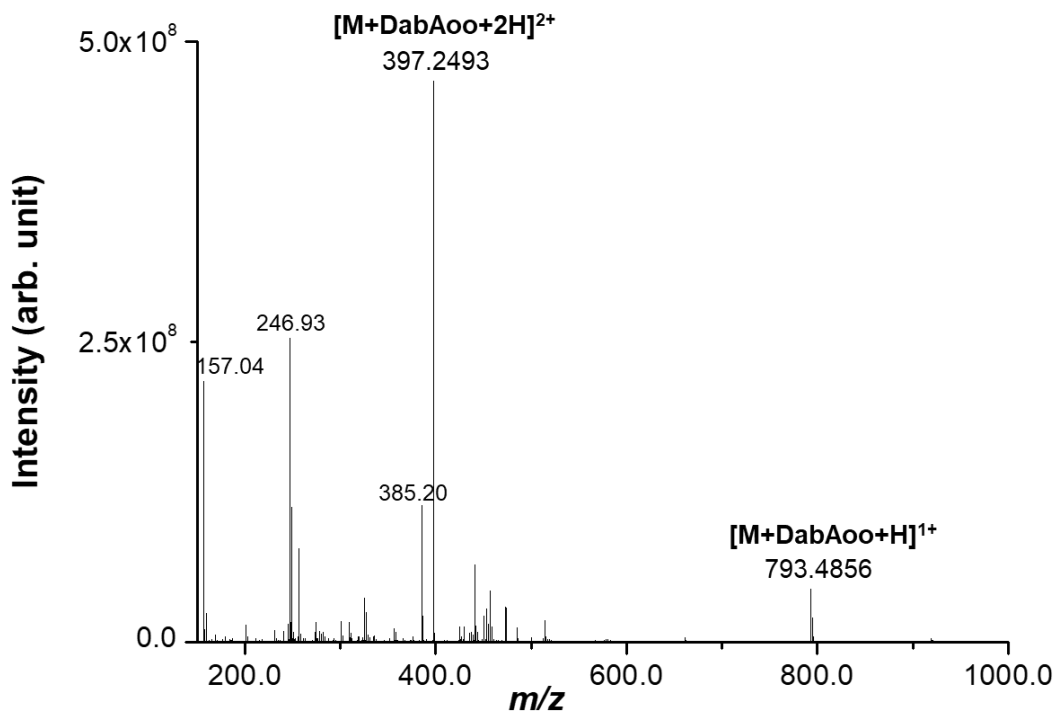


Figure S3 – Positive MS spectrum of the derivatization solution of Leupeptin with the DabAoo chromophore.

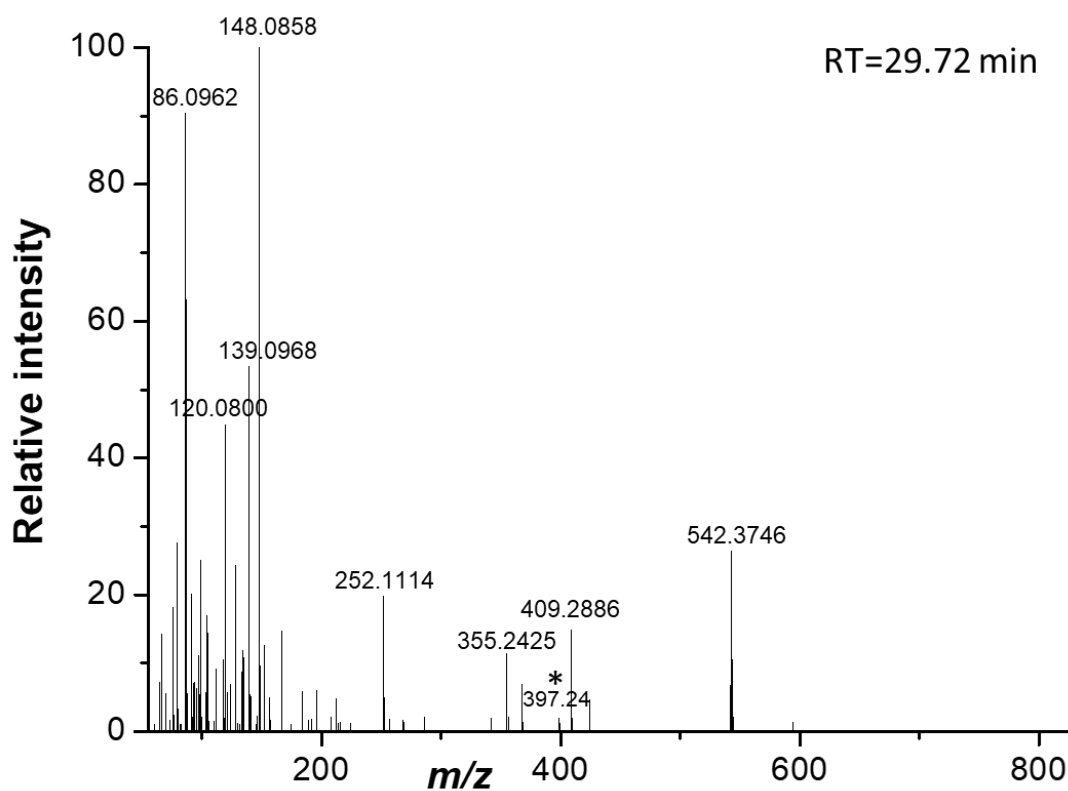


Figure S4 – LID spectrum at RT= 29.72 min of the doubly protonated derivatized leupeptin  $[M+DabAoo+2H]^{2+}$  at  $m/z$  397.24, from the top10 analysis of the derivatized leupeptine at 0.002  $\mu\text{g/mL}$  in plasma. The asterisk shows the precursor ion. All ion assignments are supported by accurate mass measurements (errors <6 ppm).

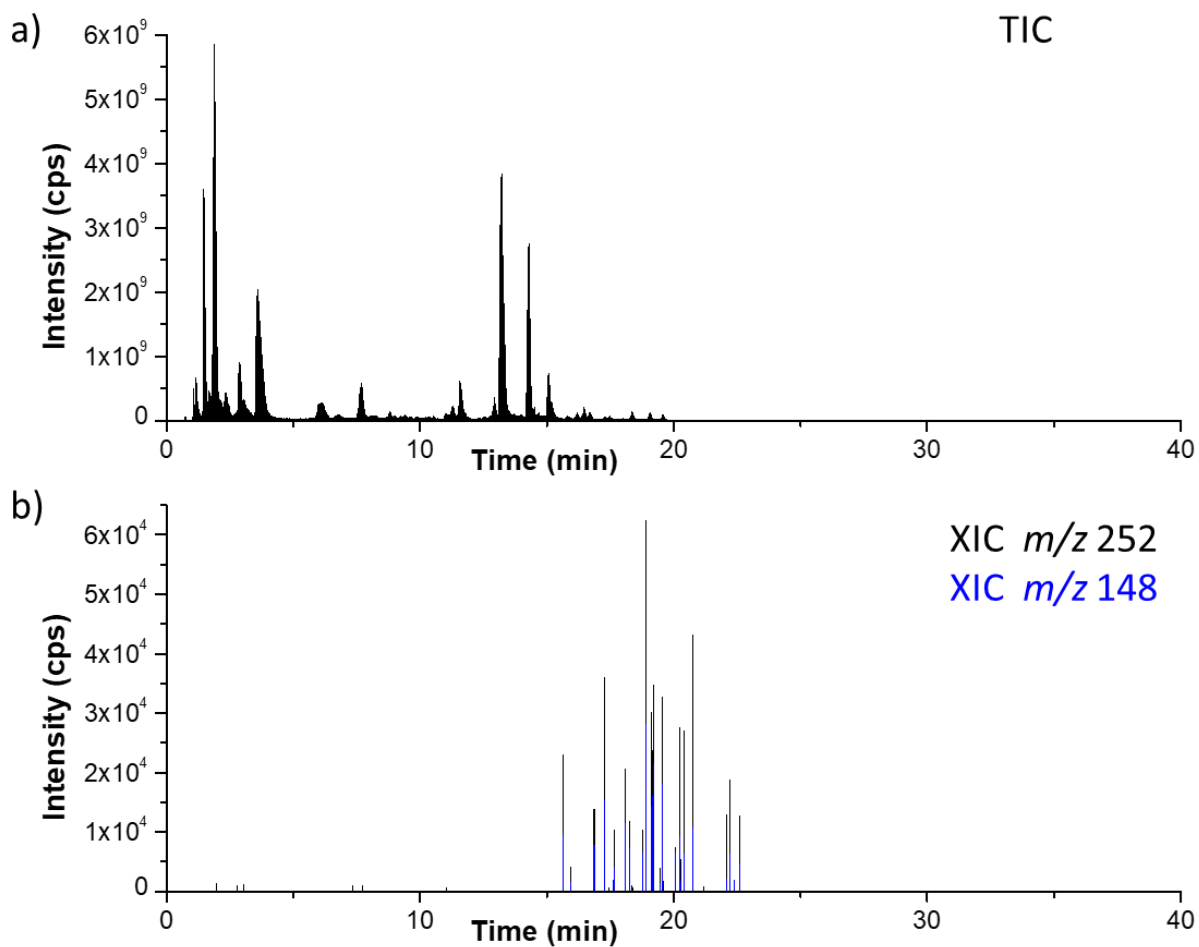


Figure S5 – a) Total ion chromatogram of the top10-LID analysis of digested derivatized MCO  $\alpha$ -syn and (b) extracted ion chromatograms of the reporter ions  $m/z$  252.11 (blue) and  $m/z$  148.01 (black).

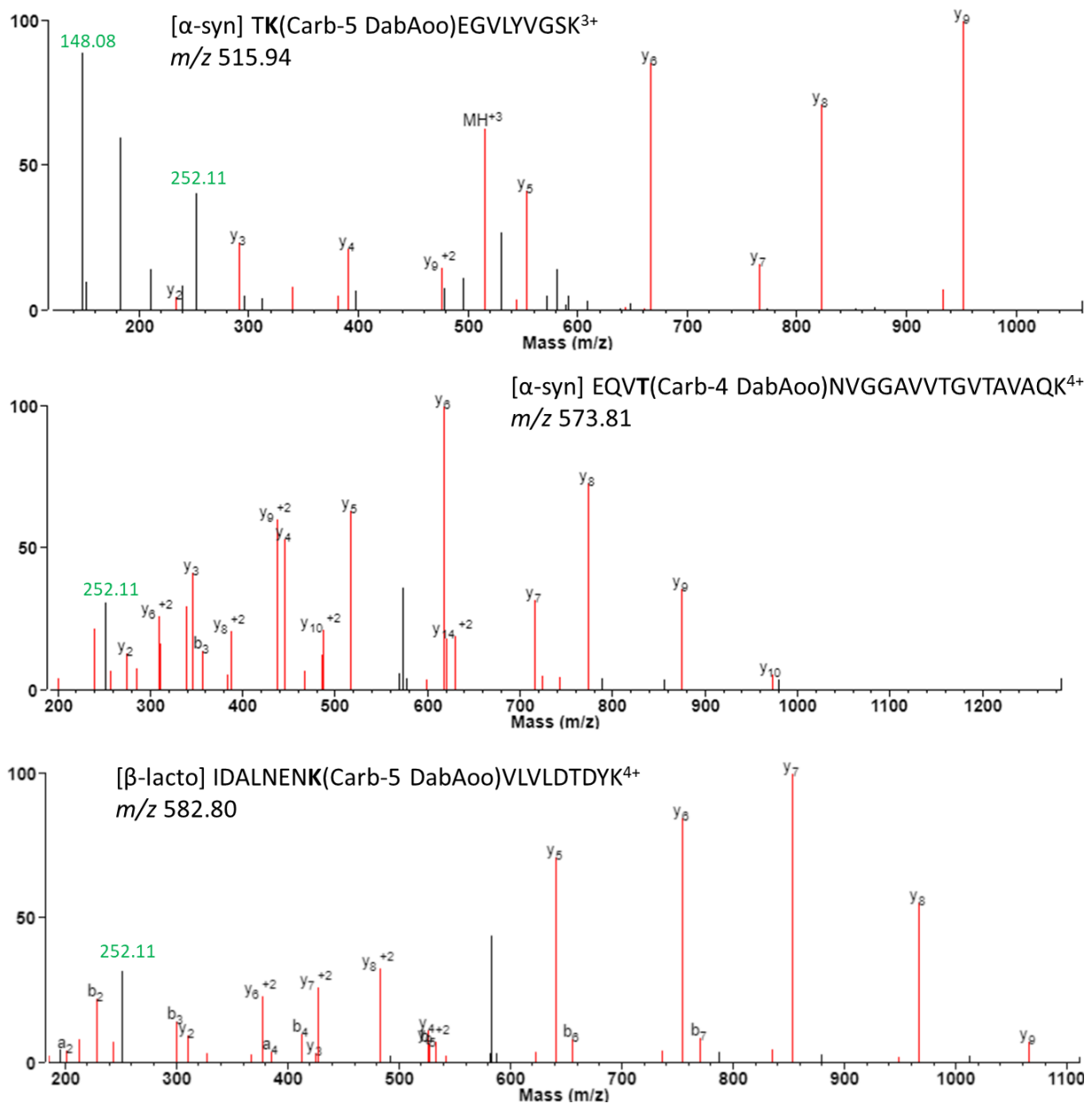


Figure S6 – LID-MS/MS of three derivatized carbonylated peptides identified by ProteinProspector from the top10-LID analysis of MCO α-syn and β-lacto samples.

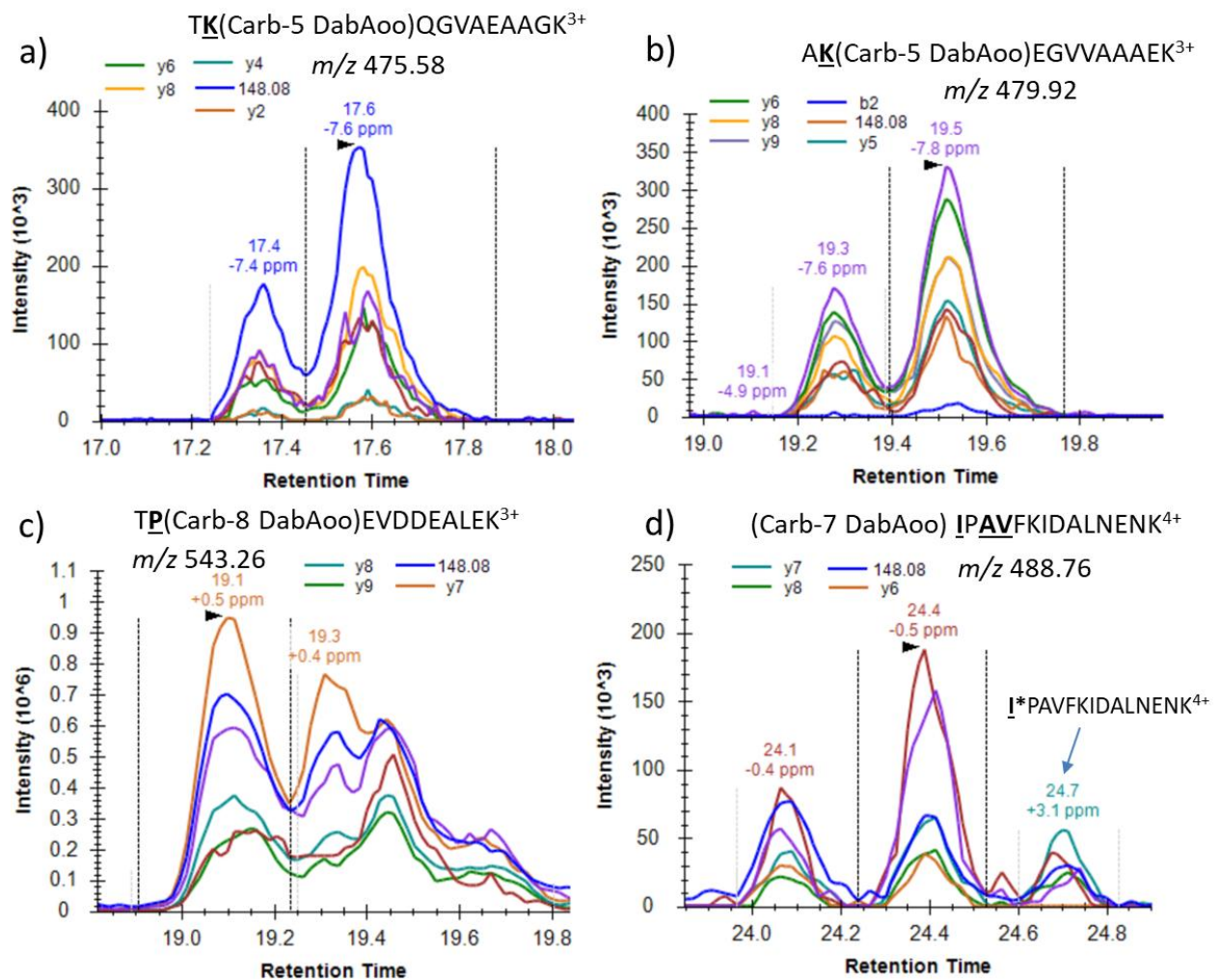


Figure S7 - Extracted ion chromatograms of fragment ions and precursor ions ( $^{12}\text{C}$  (violet line) and  $^{13}\text{C}$  isotope (red line)) detected for derivatized carbonylated peptides in MCO  $\alpha$ -syn (a and b) and  $\beta$ -lacto (c and d) samples by LID-PRM. Laser power 700 mW. The multiple peaks in a)-c) correspond to conformational stereoisomers. In d), the 3 peaks correspond to oxidation on 3 different AA sites: modification on I at 24.7 min, and undifferentiated A or V at 24.1 and 24.4 min.

Table S1: PRM precursor list of the targeted derivatized carbonylated peptides from MCO and targeted non-oxydized peptides from MCO digest  $\alpha$ -syn and  $\beta$ -lacto samples.

Protein	Peptide	<i>m/z</i>	<i>z</i>	Start Time (min)	End Time (min)
<b>Derivatized carbonylated</b>					
$\alpha$ -syn	[Carb-5 DabAoo] TVEGAGSIAAATGFVKK	658.0153	3	22.00	26.00
	TK[Carb-5 DabAoo]QGVAEAAGK	475.5794	3	16.00	19.00
	[Carb-5 DabAoo] EGVVHGVATVAEKT	630.6632	3	18.00	20.00
	[Carb-5 DabAoo] EGVVAAAETK	489.9225	3	18.00	21.00
	TK[Carb-5 DabAoo]EQVTNVGGAVVTGVTAVAQK	631.3404	4	19.50	27.50
	[Carb-4 DabAoo] TVEGAGSIAAATGFVK	461.4924	4	19.50	27.50
	[Carb-7 DabAoo] EQVTNVGGAVVTGVTAVAQK	577.8027	4	17.20	25.20
	TK[Carb-5 DabAoo]EGVVHGVATVAEK	473.2508	4	15.10	23.10
	TK[Carb-5 DabAoo]EGVLYVGSK/ EGVLYVGSK[Carb-5 DabAoo]TK	515.9400	3	18.70	26.70
	[Carb-4 DabAoo] EQVTNVGGAVVTGVTAVAQK	764.7421	3	19.00	27.00
	[Carb-7 DabAoo] EGVVHGVATVAEK	419.7166	4	12.80	20.80
	AK[Carb-5 DabAoo]EGVVAAAEEK	479.9201	3	15.50	23.50
$\beta$ -lacto	TPEVDDEALEK[Carb-5 DabAoo]FDK/ T[Carb-4 DabAoo]PEVDDEALEKFDK	500.9922	4	22.60	26.60
	[Carb-7 DabAoo] TPEVDDEALEKFDK	504.7351	4	18.30	22.30
	VYVEELK[Carb-5 DabAoo]PTPEGDLEILLQK/ VYVEELKPT[Carb-4 DabAoo]PEGDLEILLQK	670.3592	4	21.75	25.75
	VLVLDT[Carb-4 DabAoo]DYK	477.2505	3	22.30	26.30
	T[Carb-4 DabAoo]P[Carb-8 DabAoo]EVDDEALEK	498.7357	4	27.10	31.10
	IPAVFK[Carb-5 DabAoo]IDALNENK	646.3438	3	25.10	29.20
	I[Carb-7 DabAoo]PAVFK	352.1987	3	21.20	25.20
	[Carb-7 DabAoo] IDALNENKVLVLDTDYK	586.5517	4	21.10	25.10
	IDAL[Carb-7 DabAoo]NENK	432.8795	3	15.90	19.90
	ALK[Carb-5 DabAoo]ALPMHIR	379.4629	4	20.95	24.95
	[Carb-7 DabAoo] VYVEELKPTPEGDLEILLQK	674.1102	4	20.90	28.90
	[Carb-7 DabAoo] VLVLDTDYK	482.5838	3	19.00	27.00
	TP[Carb-8 DabAoo]EVDDEALEK	543.2553	3	15.40	23.40
	T[Carb-4 DabAoo]PEVDDEALEK	537.2537	3	16.00	24.00
	TPEVDDEAL[Carb-7 DabAoo] EK	542.5862	3	15.10	23.10
	[Carb-7 DabAoo] TKIPAVFK	321.6845	4	16.00	24.00
	T[Carb-4 DabAoo]KIPAVFK	423.2482	3	17.80	25.80
	[Carb-7 DabAoo] IPAVFKIDALNENK	488.7645	4	21.10	29.10
	IDALNENK[Carb-5 DabAoo]VLVLDTDYK	582.8005	4	22.50	30.50
	<b>Analogous non-carbonylated</b>				
$\alpha$ -syn	TVEGAGSIAAATGFVKK	536.2918	3	5.00	15.00
	TKQGVAEAAGK	530.2933	2	0.50	20.00
	EGVVHGVATVAEKT	508.9441	3	0.50	20.00



	EGVVAAAEKTK	368.2047	3	6.00	16.00
	EGVLYVGSKTK	394.9423	3	0.50	20.00
	TKEQVTNVGGAVVTGVTAVAQK	719.7300	3	8.00	18.00
	TVEGAGSIAAATGFVK	493.5982	3	8.00	18.00
	TKEGVVHGVATVAEK	762.9127	2	5.60	15.60
	TKEGVLYVGSK	590.8343	2	0.50	26.70
	EQVTNVGGAVVTGVTAVAQK	643.3471	3	10.10	20.20
	EGVVHGVATVAEK	648.3448	2	0.50	20.80
	AKEGVVAAAEK	536.7971	2	0.50	23.50
β-lacto	TPEVDDEALEKFDK	545.9238	3	2.00	10.00
	IPAVFK	337.7147	2	0.50	5.00
	IDALNENK	458.7349	2	12.70	16.70
	ALKALPMHIR	383.8968	3	17.70	21.70
	VYVEELKPTPEGDLEILLQK	771.7572	3	14.00	24.00
	VLVLDTDYK	355.8619	3	10.00	20.00
	TPEVDDEALEK	415.8623	3	0.50	23.10
	TKIPAVFK	301.8587	3	5.80	15.80
	IPAVFKIDALNENK	786.4381	2	21.10	29.10
	IDALNENKVLVLDTDYK	655.0137	3	9.00	19.00

Table S2. Precision and accuracy data on calibration samples for replicated derivatized leupeptin spiked at different concentration into human serum in top10-LID.

Nominal Concentration (µg/mL)	CV (%)
0.002	20
0.040	6.7
0.417	9.3
3.333	16.1

Table S3: List of peptides identified in (a) MCO and (b) control derivatized with DabAoo  $\beta$ -lactoglobulin sample, using Protein Prospector from the top10-LID analysis.

a) MCO

<i>m/z</i>	<i>z</i>	Peptide	Variable Mod @AA	RT (min)	Error ppm	Score	Expect
379.4629	4	ALKALPMHIR	Carb-5 DabAoo@3	21.55	-7.6	26.3	1.6e-08
305.1636	4	ALPMHIR	Carb-7 DabAoo@1 2	17.87	-2.7	16	1.7e-04
337.1967	2	GLDIQK		2.179	-2.6	18.4	2.5e-04
932.478	4	GLDIQKVAGTWYSLAMAASDISLLDAQ SAPLR	Carb-5 DabAoo@6	36.25	-1.3	16.6	6.6e-11
1126.5855	3	GLDIQKVAGTWYSLAMAASDISLLDAQ SAPLR	Oxidation@16	27.771	0.32	26.6	4.1e-11
432.8795	3	IDALNENK	Carb-7 DabAoo@4	15.45	-7.1	20.9	3.3e-07
655.0137	3	IDALNENKVLVLDTDYK		12.26	-5.9	19.8	2.3e-09
582.8005	4	IDALNENKVLVLDTDYK	Carb-5 DabAoo@8	24.29	-3	53.8	6.2e-14
586.5517	4	IDALNENKVLVLDTDYK	Carb-7 DabAoo@4 6	21.54	-5.5	30.8	5.5e-14
767.0827	3	IDALNENKVLVLDTDYK	Carb-3 DabAoo@6	15.02	11	18.4	1.1e-06
337.7147	2	IPIAVFK		6.401	-2.1	16.4	3.0e-04
527.793	2	IPIAVFK	Carb-7 DabAoo@1	21.63	-4.3	20.2	3.0e-06
488.7636	4	IPIAVFKIDALNENK	Carb-7 DabAoo@3 4	22.86	-3.2	29.4	4.4e-09
488.7622	4	IPIAVFKIDALNENK	Carb-7 DabAoo@1 3 4	21.66	-6.1	18.2	1.9e-08
646.3438	3	IPIAVFKIDALNENK	Carb-5 DabAoo@6	25.36	-5.7	25.1	1.6e-10
423.2482	3	TKIPIAVFK	Carb-4 DabAoo@1	20.27	-0.82	23.2	1.3e-09
301.8587	3	TKIPIAVFK		6.22	-5.2	27.8	1.0e-07
423.5761	3	TKIPIAVFK	Carb-5 DabAoo@2	22.85	-1.1	19.7	7.3e-06
321.6845	4	TKIPIAVFK	Carb-7 DabAoo@3	18.08	-7.6	18.3	5.8e-06
415.8623	3	TPEVDDEALEK		3.43	-9.7	35	8.6e-08
537.2537	3	TPEVDDEALEK	Carb-4 DabAoo@1	18.19	-1.6	34.6	8.1e-07
542.5791	3	TPEVDDEALEK	Carb-7 DabAoo@8 9	16.52	-13	29.4	4.1e-07
527.9213	3	TPEVDDEALEK	Carb-3 DabAoo@5 6 7	18.65	-3.1	21.9	4.4e-06
542.5862	3	TPEVDDEALEK	Carb-7 DabAoo@3	17.09	-0.14	25.6	8.2e-07
527.9235	3	TPEVDDEALEK	Carb-3 DabAoo@3 5 6 7	18.276	1	22.8	2.8e-06
543.2553	3	TPEVDDEALEK	Carb-8 DabAoo@2	17.44	-5.3	29.4	9.6e-08
527.9222	3	TPEVDDEALEK	Carb-3 DabAoo@10	19.47	-1.4	16	2.7e-07
498.7357	4	TPEVDDEALEK	Carb-4 DabAoo@1; Carb-8 DabAoo@2	27.49	-1.8	30.4	5.9e-08
542.5817	3	TPEVDDEALEK	Carb-7 DabAoo@4	16.89	-8.4	19.2	2.4e-06
504.7361	4	TPEVDDEALEKFDK	Carb-7 DabAoo@3 4	18.87	-6	37.9	2.7e-10
493.7396	4	TPEVDDEALEKFDK	Carb-3 DabAoo@10	19.84	-4.2	25.6	2.6e-08

500.9822	4	TPEVDDEALEKFDK	Carb-5 DabAoo@11	22.42	-8.3	32.5	1.3e-10
500.741	4	TPEVDDEALEKFDK	Carb-4 DabAoo@1	19.23	1.3	25.5	1.2e-08
504.7351	4	TPEVDDEALEKFDK	Carb-7 DabAoo@9 10	18.52	-8	20.8	2.8e-07
504.737	4	TPEVDDEALEKFDK	Carb-7 DabAoo@3 10	18.56	-4.2	24.2	2.8e-07
493.7386	4	TPEVDDEALEKFDK	Carb-3 DabAoo@7 10	19.11	-6.2	15.6	4.3e-06
1024.5176	3	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-4 DabAoo@4 7	32.08	-0.86	35.4	2.7e-17
1030.52	3	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-8 DabAoo@24	29.70	-1.9	17.6	8.0e-07
761.6373	4	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-3 DabAoo@14	30.91	-6.1	41	8.6e-14
1126.5855	3	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-2 DabAoo@10; Carb-3 DabAoo@14	27.77	7.2	26.1	9.4e-11
1024.5142	3	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-4 DabAoo@7 13	29.95	-4.2	32.1	6.4e-14
1151.2304	3	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-7 DabAoo@12; Carb-4 DabAoo@13	30.92	-6.9	27.4	2.2e-13
1029.8454	3	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-7 DabAoo@25	30.07	-4.5	27.9	4.9e-09
1136.5655	3	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-3 DabAoo@14; Carb-4 DabAoo@4 7 13	29.88	-8.4	29.2	4.8e-12
1024.5118	3	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-4 DabAoo@16	31.40	-6.5	25.9	5.6e-12
785.1471	4	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-10 DabAoo@5&Oxidation@10   Carb-11 DabAoo@5	27.11	9.8	19.5	2.1e-10
1041.1948	3	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-10 DabAoo@5  Carb-9 DabAoo@5 6&Oxidation@10	29.90	9.2	20.4	4.6e-10
768.6348	4	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-4 DabAoo@13 16 22	30.93	-7.6	31.2	1.4e-11
1029.8454	3	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-7 DabAoo@25	30.07	-4.5	27.9	1.3e-11
1029.8421	3	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-7 DabAoo@1 2 11 12 15	29.35	-7.7	26.4	5.1e-11
1029.8455	3	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-7 DabAoo @1 2 5 6 8 9 11 12	30.44	-4.4	26.2	3.2e-08
868.6762	4	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-11 DabAoo@5; Carb-2 DabAoo@10	32.30	-7.2	20.2	3.3e-11
785.1471	4	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-11 DabAoo@5	27.11	9.8	19.5	2.2e-07
772.6392	4	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-7 DabAoo@1 2 5 6 8 9 11 1 2 15	28.81	-0.26	20.9	2.4e-07
856.1896	4	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-2 DabAoo@10;Carb-7 DabAoo@1 2 5 6 8 9 11 1 2 15	30.80	8.5	16.7	2.9e-10
1041.1948	3	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-10 DabAoo@5	29.90	9.2	20.4	4.1e-07
1141.8935	3	VAGTWYSLAMAASDISLLDAQSAPLR	Carb-3 DabAoo@14;Carb-7 DabAoo@1 2 5 6 8 9 11 1 2 15	28.49	-12	18.5	5.1e-08
355.8619	3	VLVLDTDYK		8.61	-11	21.1	1.1e-08
477.2505	3	VLVLDTDYK	Carb-4 DabAoo@6	22.43	-7.3	29.2	2.4e-07
482.5853	3	VLVLDTDYK	Carb-7 DabAoo@1 2 3	20.93	-0.74	15.6	1.1e-05
467.9192	3	VLVLDTDYK	Carb-3 DabAoo@5 7	22.20	-6.7	15	2.8e-06

482.5838	3	VLVLDTDYK	Carb-7 DabAoo@3 4	20.12	-3.9	15.6	1.7e-05
398.5656	3	VLVLDTDYKK		5.99	3.9	17.3	6.8e-08
394.2126	4	VLVLDTDYKK	Carb-7 DabAoo@1 2 3 4	18.61	-5.7	22.3	4.9e-07
520.277	3	VLVLDTDYKK	Carb-5 DabAoo@9	22.09	-6.4	22.7	1.9e-09
394.2117	4	VLVLDTDYKK	Carb-7 DabAoo@1 2 3 4	17.86	-7.9	19.4	9.3e-08
394.2143	4	VLVLDTDYKK	Carb-7 DabAoo@1 2 3	19.28	-1.3	22.6	1.6e-06
771.7572	3	VYVEELKPTPEGDLEILLQK		17.00	-0.78	33.9	3.9e-12
663.1111	4	VYVEELKPTPEGDLEILLQK	Carb-3 DabAoo@11	24.95	-2.3	35	3.9e-10
674.1049	4	VYVEELKPTPEGDLEILLQK	Carb-7 DabAoo@4 5 6	24.81	-7.8	39.2	2.1e-12
663.1122	4	VYVEELKPTPEGDLEILLQK	Carb-3 DabAoo@4 5	24.21	-0.69	46.2	5.5e-14
674.1102	4	VYVEELKPTPEGDLEILLQK	Carb-7 DabAoo@16 17	22.94	0.12	31.7	2.8e-10
670.1099	4	VYVEELKPTPEGDLEILLQK	Carb-4 DabAoo@9	24.30	-2.2	43	1.2e-12
670.3592	4	VYVEELKPTPEGDLEILLQK	Carb-5 DabAoo@7	27.92	2.7	38.4	4.2e-12
674.1097	4	VYVEELKPTPEGDLEILLQK	Carb-7 DabAoo@11	23.91	-0.63	35	9.9e-11
674.1054	4	VYVEELKPTPEGDLEILLQK	Carb-7 DabAoo@1 3 4 5 6	25.16	-7	31.1	3.8e-10
765.6497	4	VYVEELKPTPEGDLEILLQK	Carb-4 DabAoo@9; Carb-8 DabAoo@8 10	30.93	-7.1	27.6	2.4e-09
674.6044	4	VYVEELKPTPEGDLEILLQK	Carb-8 DabAoo@8 10	24.46	-14	27.9	1.0e-06
899.1418	3	VYVEELKPTPEGDLEILLQK	Carb-8 DabAoo@8 10	24.25	-8.6	26.2	1.8e-09
883.8051	3	VYVEELKPTPEGDLEILLQK	Carb-3 DabAoo@11 13 15	24.33	-11	21.7	4.9e-08
674.1045	4	VYVEELKPTPEGDLEILLQK	Carb-7 DabAoo@14 15 16	22.29	-8.3	20.4	1.0e-07
898.4773	3	VYVEELKPTPEGDLEILLQK	Carb-7 DabAoo@11 14 15 16	25.31	-0.41	17.9	5.4e-05

b) Control

<i>m/z</i>	<i>z</i>	Peptide	Variable Mod @AA	RT (min)	Error ppm	Score	Expect
771.7477	3	VYVEELKPTPEGDLEILLQK		19.31	-13	40.9	8.6e-13
533.2876	2	VLVLDTDYK		7.86	-14	16.5	1.1e-09
415.8603	3	TPEVDDEALEK		1.045	-14	50.5	6.8e-09
398.5627	3	VLVLDTDYKK		1.72	-3.4	32.9	2.1e-08
458.7339	2	IDALNENK		1.249	-14	15	1.4e-05
337.7127	2	IPAVFK		4.11	-8	21.7	3.2e-05

Table S4: List of peptides identified in control  $\alpha$ -synuclein sample derivatized with DabAoo, using Protein Prospector from the top10-LID analysis.

<i>m/z</i>	<i>z</i>	Peptide	Variable Mod @AA	RT (min)	Error ppm	Score	Expect
1434.8952	3	NEEGAPQEGILEDMPVDPDNEA YEMPSEEGYQDYEPEA	Oxidation@14	16.791	-13	31.7	7.6e-25
1076.424	4	NEEGAPQEGILEDMPVDPDNEA YEMPSEEGYQDYEPEA	Oxidation@25	18.497	-13	24.1	2.7e-15
493.5954	3	TVEGAGSIAAATGFVK		13.334	-9.1	53.3	4.6e-13
393.6749	2	MDVFMK	Oxidation@5	1.775	-13	18.4	3.7e-12
719.7249	3	TKEQVTNVGGAVVTGVTAVAQK		12.816	-13	33.3	6.6e-12
1080.4223	4	NEEGAPQEGILEDMPVDPDNEA YEMPSEEGYQDYEPEA	Oxidation@14;Oxidation@25	15.341	-13	16	1.6e-11
479.9145	3	AKEGVVAAAEEK	Carb-5 DabAoo@2	19.525	-14	16.7	1.1e-09
643.3445	3	EQVTNVGGAVVTGVTAVAQK		12.243	-13	26	1.5e-09
476.2579	2	EGVLYVGSK		1.801	-6.3	17.7	3.1e-08
394.2182	3	TKEGVLYVGSK		1.008	-15	36.9	4.8e-08
432.5664	3	EGVVHGVATVAEK		1.22	-8.4	28.4	9.3e-08
385.6799	2	MDVFMK		8.251	-6.4	18.9	1.3e-07
415.7161	2	QGVAAEAGK		1.019	-14	17.8	5.5e-07
437.2323	2	EGVAAAEEK		1.478	-12	17.2	1.4e-06
406.6818	2	MDVFMK	Acetyl@N-term	17.439	-14	19.6	8.0e-06

Table S5: Oxidative ratio of detected carbonylated peptides quantified in MCO  $\alpha$ -synuclein and  $\beta$ -lactoglobulin samples derivatized with DabAoo.

<b>Protein</b>	<b>Peptide</b>	<b>Oxidative ratio</b>
$\alpha$ -syn	[Carb-5 DabAoo] TVEGAGSIAAATGFVKK	0.03030
	TK[Carb-5 DabAoo]QGVAAEAGK	2.70019
	[Carb-5 DabAoo] EGVVHGVATVAEKT	0.05455
	[Carb-5 DabAoo] EGVVAAAEKTK	0.98851
	TK[Carb-5 DabAoo]EQVTNVGGAVVTGVTAVAQK	0.00121
	[Carb-4 DabAoo] TVEGAGSIAAATGFVK	0.00005
	[Carb-7 DabAoo] EQVTNVGGAVVTGVTAVAQK	0.00012
	TK[Carb-5 DabAoo]EGVVHGVATVAEK	2.21413
	TK[Carb-5 DabAoo]EGVLYVGSK	0.31777
	EGVLYVGSK[Carb-5 DabAoo]TK	0.60214
	[Carb-4 DabAoo] EQVTNVGGAVVTGVTAVAQK	0.00095
	[Carb-7 DabAoo] EGVVHGVATVAEK	0.00149
	AK[Carb-5 DabAoo]EGVVAAAEK	1.08995
$\beta$ -lacto	TPEVDDEALEK[Carb-5 DabAoo]FDK/ T[Carb-4 DabAoo]PEVDDEALEKFDK	0.00298
	[Carb-7 DabAoo] TPEVDDEALEKFDK	0.03659
	VYVEELK[Carb-5 DabAoo]PTPEGDLEILLQK/ VYVEELKPT[Carb-4 DabAoo]PEGDLEILLQK	0.00883
	VLVLDT[Carb-4 DabAoo]DYK	1.14615
	T[Carb-4 DabAoo]P[Carb-8 DabAoo]EVDDEALEK	0.00993
	IPAVFK[Carb-5 DabAoo]IDALNENK	0.51908
	I[Carb-7 DabAoo]PAVFK	0.00777
	[Carb-7 DabAoo] IDALNENKVLVLDTDYK	1.56757
	IDAL[Carb-7 DabAoo]NENK	0.00080
	ALK[Carb-5 DabAoo]ALPMHIR	0.01708
	[Carb-7 DabAoo] VYVEELKPTPEGDLEILLQK	0.02507
	[Carb-7 DabAoo] VLVLDTDYK	1.09231
	TP[Carb-8 DabAoo]EVDDEALEK	0.20144
	T[Carb-4 DabAoo]PEVDDEALEK	0.31367
	TPEVDDEAL[Carb-7 DabAoo] EK	0.24964
	[Carb-7 DabAoo] TKIPAVFK	0.04483
	T[Carb-4 DabAoo]KIPAVFK	0.04172
	[Carb-7 DabAoo] IPAVFKIDALNENK	1.84733
	IDALNENK[Carb-5 DabAoo]VLVLDTDYK	0.44515

Top10 analysis and search results can be accessed here:

$\beta$ -lactoMCO

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$\beta$ -lactoCtl

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$\alpha$ -synMCO

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$\alpha$ -synCtl

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