Supplementary Material

The NMR signature of maltose-based glycation in full-length proteins

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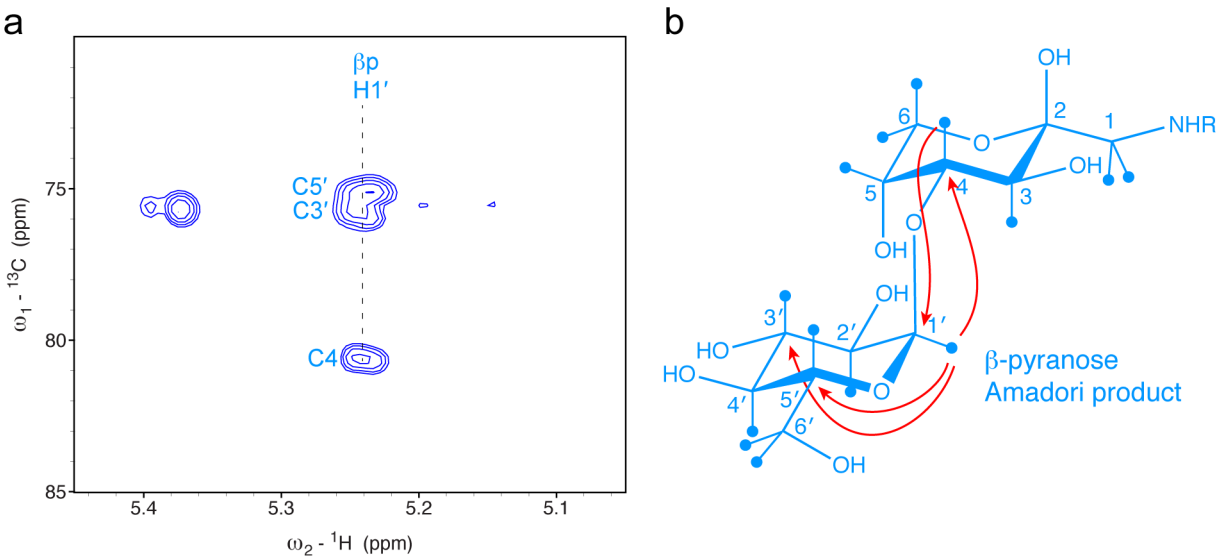
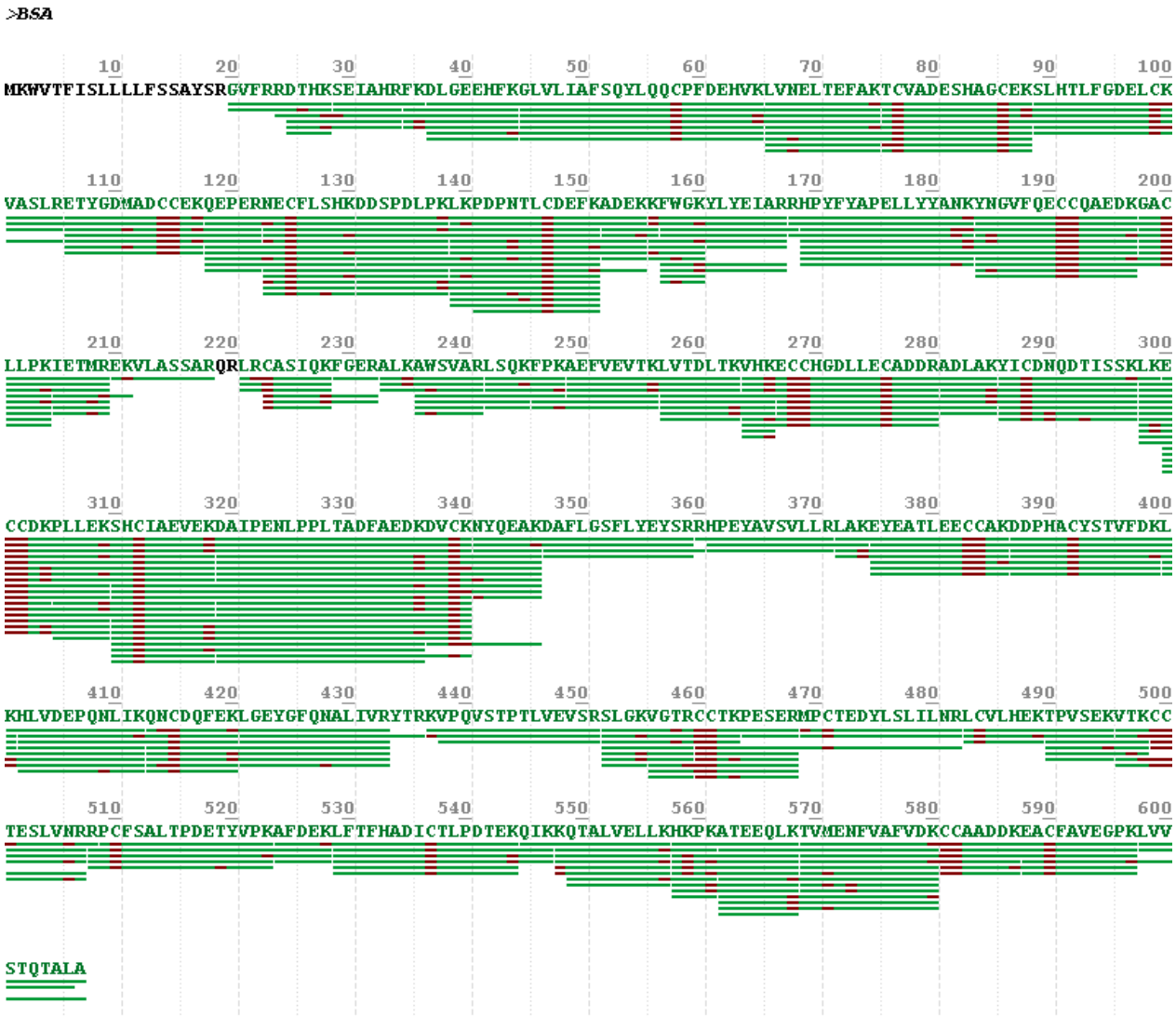
Supplementary Figures



Supplementary Figure S1. Observed ^{1}H-^{13}C long-range correlations of the major form of the glycation product of BSA with maltose. a) Part of a 2D ^{1}H-^{13}C HMBC spectrum showing correlations to the anomeric H1 of the distal glucose of the major β-pyranose form.



Supplementary Figure S2. Coverage of the BSA sequence by the MS/MS analysis. Identified peptides are indicated in green, modified amino acids are shown in red (e.g. with glycated Lys, alkylated Cys, deamidation, phosphorylation or oxidation).

Supplementary Figure S3. Graphical representation of the BSA (Uniprot ID P02769) sequence coverage. The areas in green were identified in one or more peptides, with a total sequence coverage of 96.5%, black areas were not identified. Red underlined lysine residues were identified with a +324 Da modification corresponding to glycation with maltose.

Supplementary Tables

Table S1 Observed peptide fragments in the MS/MS analysis.

Peptides containing Lysine residues	Residue	Maltosylation [%] ± C.I. 95% (n=5)
DTHKSEIAHR	K(28)	78.4 ± 5.0
FKDLGEEHFK	K(36)	3.2 ± 0.4
DLGEEHFKGLVLIAFSQYLQQCPFDEHVK	K(44)	0.7 ± 0.6
GLVLIAFSQYLQQCPFDEHVKLVNELTEFAK	K(65)	63.8 ± 26.2
LVNELTEFAKTCVADESHAGCEK	K(75)	77.0 ± 2.4
TCVADESHAGCEKSLHTLFGDELCK	K(88)	75.6 ± 0.8
SLHTLFGDELCKVASLR	K(100)	35.6 ± 4.0
ETYGDMADCCEKQEPER	K(117)	80.3 ± 2.8
NECFLSHKDDSPDLPK	K(130)	1.4 ± 0.6
DDSPDLPKLKPDPNTLCDEFK	K(138)	3.7 ± 1.2
LKPDPNTLCDEFK	K(140)	3.4 ± 2.9
PDPNTLCDEFK	K(151)	0 ± 0
ADEKKFWGK	K(155)	0 ± 0
KFWGKYLYEIAR	K(156)	98.2 ± 0.5
FWGKYLYEIAR	K(160)	89.6 ± 0.5
HPYFYAPELLYYANKYNGVFQECCQAEDK	K(183)	57.3 ± 9.6
YNGVFQECCQAEDKGACLLPK	K(197)	56.1 ± 5.2
GACLLPKIETMR	K(204)	58.6 ± 6.2
GACLLPKIETMREK	K(211)	0 ± 0
LRCASIQK	K(228)	0 ± 0
ALKAWSVAR	K(235)	93.2 ± 3.7
AWSVARLSQK	K(245)	0 ± 0
FPKAEFVEVTK	K(248)	73.9 ± 2.7
AEFVEVTKLVTDLTK	K(256)	75.8 ± 4.9
LVTDLTKVHK	K(263)	32.8 ± 7.2
VHK(1)ECCHGDLLECADDR	K(266)	74.5 ± 0.7
ADLAKYICDNQDTISSK	K(285)	86.7 ± 2.5
YICDNQDTISSKLK	K(297)	47.1 ± 4.5
LKECCDKPLLEK	K(299)	9.5 ± 3.4
ECCDKPLLEK	K(304)	3.1 ± 1.3
PLLEKSHCIAEVEK	K(309)	5.3 ± 2.6
SHCIAEVEKDAIPENLPPLTADFAEDKDVCK	K(318)	1.4 ± 0.5
SHCIAEVEKDAIPENLPPLTADFAEDKDVCK	K(336)	0.4 ± 0.4
DVCKNYQEAK	K(340)	1.5 ± 0.9

NYQEAKDAFLGSFLYEYSR	K(346)	86.7 ± 21.7
LAKEYEATLEECCAK	K(374)	82.9 ± 1.8
EYEATLEECCAKDDPHACYSTVFDK	K(386)	47.2 ± 4.1
DDPHACYSTVFDKLK	K(399)	87.9 ± 1.8
LKHLVDEPQNLIK	K(401)	80.1 ± 5.5
HLVDEPQNLIKQNCDQFEK	K(412)	81.8 ± 5.3
QNCDQFEKLGEYGFQNALIVR	K(420)	89.8 ± 1.9
KVPQVSTPTLVEVSR	K(437)	1.8 ± 0.2
SLGKVGTR	K(455)	83.5 ± 1.1
CCTKPESER	K(463)	4.5 ± 1.0
LCVLHEKTPVSEK	K(489)	80.7 ± 3.6
TPVSEKVTKCCTESLVNR	K(495)	62.4 ± 41.1
VTKCCTESLVNR	K(498)	31.6 ± 6.2
RPCFSALTPDETYVPKAFDEK	K(523)	95.4 ± 1.8
AFDEKLFTFHADICTLPDTEK	K(528)	90.5 ± 1.9
LFTFHADICTLPDTEKQIK	K(544)	0 ± 0
LFTFHADICTLPDTEKQIK	K(547)	0 ± 0
KQTALVELLK	K(548)	36.5 ± 1.4
QTALVELLK	K(557)	0 ± 0
HKPKATEEQLK	K(559)	57.0 ± 7.3
HKPKATEEQLK	K(561)	63.7 ± 56.7
ATEEQLKTVMENFVAFVDK	K(568)	2.8 ± 0.7
TVMENFVAFVDKCCAADDKEACFAVEGPK	K(580)	8.9 ± 3.1
CCAADDKEACFAVEGPK	K(587)	0.4 ± 0.1
EACFAVEGPKLVVSTQTALA	K(597)	0.4 ± 0.1
	Total	41.8 ± 4.6