

Supplemental Information

Table 1. Modified peptides identified in tryptic digests of minimally glycosylated HSA

Observed mass for collected peptides at given % acetonitrile (ACN) in water					Predicted mass	Residues (Δ M)	Type of modification ^a	Modified residues
5% ACN	10% ACN	20% ACN	30% ACN	50% ACN				
955.49	955.52				955.5470	219-225 (+80.0266)	Argpyrimidine	R222
971.54					971.5527	535-541 (+162.0528)	FL	K536 or K538
				1820.00	1819.9701	191-205 (+144.0423)	FL-1 H ₂ O or 3-DG-H1 or THP	K195, K199 or R197
				2045.08	2045.0339	196-209 (+324.1057)	2 FL	K199 & K205
				2162.03	2162.0333	467-484 (+39.9949)	G-H1	R472
			2163.06		2163.1180	145-160 (+108.0211)	Pyrraline	K159
				2466.26	2466.2240	200-218 (+270.0740)	AFGP	K205, R209 or K212
			2612.22		2612.2423	160-181 (+39.9949)	G-H1	R160
				2651.30	2651.4298	219-240 (+144.0423)	FL-1 H ₂ O or 3-DG-H1 or THP	K225, K233 or R222
				2974.40	2974.3273	349-372 (+144.0423)	FL-1 H ₂ O	K351 or K359

^aSee Figure 1 for the full names and structures of these various modification classes.

Supplemental Information

Table 2. Non-modified peptides identified in tryptic digests of minimally glycosylated HSA

Observed mass w/o fractionation	Observed mass for collected peptides At given % acetonitrile (ACN) in water					Predicted mass ^a	Residues
	5% ACN	10% ACN	20% ACN	30% ACN	50% ACN		
673.38	645.34					645.3572	182-186
	673.37	673.38				673.3785	213-218
	695.37					695.3364	318-323
	772.43					772.4391	175-181
	789.45					789.4723	234-240
	880.43					880.4416	226-233
927.49	927.49	927.49	927.49			927.4940	138-144
933.51	933.51	933.52	933.52			933.5192	74-81
940.44	940.44					940.4488	107-114
	951.46					951.4424	13-20
960.56	960.56	960.56	960.56			960.5631	403-410
	984.52	984.53				984.4891	352-359
1055.60		1000.60				1000.6044	526-534
	1017.52	1017.53				1017.5370	65-73
	1055.54	1055.59				1055.5890	137-144
	1074.53					1074.5432	182-190
	1075.48	1075.51				1075.4995	99-106
		1128.69				1128.6992	525-534
1138.53	1138.49					1138.4984	476-484
1149.61	1149.61	1149.62	1149.61			1149.6156	42-51
	1226.60	1226.61				1226.6058	11-20
1311.74				1250.67		1250.6350	429-439
			1311.75	1311.75		1311.7425	338-348
1342.65			1342.65	1342.64	1342.62	1342.6352	546-557
	1371.54	1371.56				1371.5672	163-174
	1400.66	1400.66				1400.6779	433-444
	1434.54	1434.54				1434.5339	82-93
	1443.62	1443.64				1443.6425	263-274
1467.85			1467.84	1467.84	1467.84	1467.8436	337-348
1511.87		1511.85	1511.85			1511.8434	415-428
	1546.72	1546.73				1546.7975	275-286
	1552.62					1552.5981	360-372
1623.76					1623.77	1623.7881	324-336
	1627.71				1627.77	1627.7274	561-574
					1639.79	1639.7830	324-336 (Met-ox)
1639.94		1639.94	1639.94			1639.9384	414-428
1657.75		1657.76	1657.75	1657.75		1657.7533	390-402
1714.80	1714.79	1714.80				1714.7972	94-106
				1742.83	1742.86	1742.8947	146-159
1898.94				1898.96	1898.98	1898.9958	145-159 or 146-160
			1910.92	1910.90	1910.90	1910.9322	485-500
				1932.03		1932.0378	65-81
2045.09			2045.12	2045.10	2045.08	2045.0961	373-389
2086.85	2086.87	2086.84	2086.84			2086.8379	241-257
2260.04				2260.03	2260.02	2260.0232	501-519

Table 2. Non-modified peptides identified in tryptic digests of minimally glycosylated HSA (Cont'd)

Observed mass w/o fractionation	Observed mass for collected peptides At given % acetonitrile (ACN) in water					Predicted mass ^a	Residues
	5% ACN	10% ACN	20% ACN	30% ACN	50% ACN		
				2289.00		2289.0717	542-560
		2305.10		2305.07		2305.0666	542-560 (Met-ox)
						2490.2894	2490.2856
						2518.2383	2518.2144
		2650.28		2650.27		2650.2645	115-136
					2674.32	2674.3155	445-466
				2778.38		2778.3595	115-137
				2974.43	2974.40	2974.3449	287-313

Supplemental Information

Table 3. Modified peptides identified in Glu-C digests of minimally glycosylated HSA

Observed mass for collected peptides at given % acetonitrile (ACN) in water ^a					Predicted mass	Residues (ΔM)	Type of modification ^a	Modified residues
5% ACN	10% ACN	20% ACN	30% ACN	50% ACN				
858.45					858.4614	377-382 (+126.0317)	FL-2 H ₂ O	K378
933.46					933.4934	377-383 (+72.0211)	CEL	K378
1130.56	1130.56				1130.5152	286-294 (+58.0055)	CML	K286
			1166.58		1166.5039	49-57 (+126.0317)	FL-2 H ₂ O	K51
1348.72					1348.7042	133-141 (+144.0423)	FL-1 H ₂ O	K136 or K137
1434.79					1434.8319	572-585 (+108.0211)	Pyrraline	K573 or K574
		1462.75			1462.7178	7-17 (+162.0528)	FL	K12
			1866.99		1867.0006	154-167 (+162.0528)	FL	K159 or K162
2118.07	2118.05				2118.0436	426-442 (+162.0528)	FL	K432, K436 or K439
		2194.16			2194.0856	377-393 (+108.0211)	Pyrraline	K378 or K389
			2548.33		2548.1845	168-188 (+72.0211)	CEL	K174 or K181

^aSee Figure 1 for the full names and structures of these various modification classes.

Supplemental Information

Table 4. Non-modified peptides identified in Glu-C digests of minimally glycosylated HSA

Observed mass w/o fractionation	Observed mass for collected peptides At given % acetonitrile (ACN) in water					Predicted mass	Residues
	5% ACN	10% ACN	20% ACN	30% ACN	50% ACN		
962.48	962.46					962.4552	443-450
		978.48				978.4501	443-450 (Met-ox)
1031.46	1031.44	1031.44				1031.4507	369-376
	1197.56	1197.56				1197.5792	496-505
1204.65				1204.66		1204.6619	133-141
	1213.53					1213.5522	312-321
	1278.79					1278.7900	532-542
1300.67	1300.66	1300.66	1300.66			1300.665	7-17
	1313.79	1313.79				1313.7907	521-531
1326.80						1326.8108	572-585
1519.78	1519.79	1519.78	1519.78	1519.78		1519.781	142-153
	1541.77	1541.77	1541.77			1541.6946	506-518
1548.80	1548.77	1548.81	1548.80	1548.80		1548.7956	480-492
1566.65		1566.62				1566.6203	120-132
1583.78				1583.83		1583.7883	543-556
	1680.80	1680.81				1680.8049	466-479
1699.77			1699.75			1699.7418	253-266
1704.95	1704.96		1704.96	1704.95	1704.95	1704.9478	154-167
1737.71	1737.69	1737.71				1737.6994	87-100
1801.89					1801.90	1801.9158	451-465
1955.99	1955.99	1955.98				1955.9908	426-442
2086.06			2086.06	2086.09		2086.0645	377-393
2194.20		2194.12	2194.16			2194.1768	189-208
2232.25			2232.21	2232.25	2232.25	2232.2518	209-227
2348.20			2348.19	2348.24		2348.1934	101-119
2563.43					2563.38	2563.4149	334-354
2578.31				2578.31		2578.2758	61-82
					2745.31	2745.3526	443-465
				2922.59		2922.6459	401-425
					3334.62	3334.7299	18-45

Supplemental Information

Table 5. Modified peptides identified in Lys-C digests of minimally glycosylated HSA

Observed mass for collected peptides at given % acetonitrile (ACN) in water					Predicted mass	Residues (ΔM)	Type of modification ^a	Modified residues
5% ACN	10% ACN	20% ACN	30% ACN	50% ACN				
	873.52				873.5159	520-525 (+72.0211)	CEL	K524 or K525
			2527.38		2527.3574	206-225 (+162.0528)	FL	K212 or K225

^aSee Figure 1 for the full names and structures of these various modification classes.

Supplemental Information

Table 6. Non-modified peptides identified in Lys-C digests of minimally glycosylated HSA

Observed mass w/o fractionation	Observed mass for collected peptides at given % acetonitrile (ACN) in water					Predicted mass ^a	Residues
	5% ACN	10% ACN	20% ACN	30% ACN	50% ACN		
673.42	599.39					599.3768	282-286
	673.40					673.3997	520-524
	772.44					772.4391	175-181
	784.39					784.3881	373-378
854.46	789.47					789.4721	234-240
	854.46	854.45	854.48			854.4525	206-212
	880.45					880.4416	226-233
	951.44					951.4424	13-20
973.54	973.52	973.52				973.5219	5-12
	1000.58	1000.59				1000.6044	526-534
	1002.57					1002.5583	467-475
	1017.54	1017.53	1017.55			1017.5370	65-73
	1070.46					1070.4464	565-573
	1074.54					1074.5431	182-190
1149.61	1128.70					1128.6994	525-534
	1149.61	1149.61	1149.62			1149.6156	42-51
	1198.54					1198.5414	565-574
	1279.71	1279.71	1279.71			1279.7261	379-389
1342.63	1342.64	1342.64	1342.63	1342.63	1342.6352	546-557	
1352.77	1352.76	1352.77	1352.77	1352.77		1352.7691	403-413
	1371.56	1371.57				1371.5672	163-174
	1443.64	1443.66				1443.6425	263-274
			1480.84			1480.8641	403-414
1529.87	1529.87	1529.87	1529.87	1529.87	1529.86	1529.8705	213-225
	1552.60					1552.5981	360-372
1657.75	1657.75	1657.76	1657.74	1657.75		1657.7533	390-402
1714.78	1714.80	1714.80	1714.78			1714.7972	94-106
1827.94	1827.97	1827.95	1827.93			1827.9640	175-190
1924.07		1924.08	1924.06	1924.08		1924.0869	415-432
2045.10			2045.05	2045.12		2045.0961	373-389
2052.16	2052.20		2052.15			2052.1819	414-432
				2067.10		2067.1287	196-212
			2075.91			2075.8836	558-574
2260.02				2260.07	2260.03	2260.0232	501-519
2349.03			2348.98	2349.04	2349.06	2349.0347	74-93
2391.27				2391.37		2391.2937	213-233
2490.22					2490.26	2490.2856	21-41
2585.10	2585.10	2585.11	2585.06			2585.1181	241-262
2674.30				2674.35	2674.32	2674.3155	445-466
					2690.33	2690.3104	445-466 (Met-ox)
2807.44				2807.47	2807.47	2807.4714	138-159
2935.58				2935.59	2935.57	2935.5664	137-159
2974.34				2974.41	2974.41	2974.3449	287-313
3030.50				3030.57		3030.4122	476-500