Supplementary Information

Chemokine Binding to PSGL-1 is Controlled by O-Glycosylation and Tyrosine Sulfation

Supplementary Figure Legends

Figure S1. Thr44 of PSGL-1 is O-glycosylated. Related to Figure 1, 2.

a) MALDI spectrum showing the mass of unmodified PSGL-1 peptide and glycosylated peptide. After incubation with GalNAc-T1, there are three peaks corresponding to the unmodified starting peptide, the peptide with one GalNAc- attached and the peptide with two GalNAc attached. b) The novel site of human Thr44 is located closer to the sulfated tyrosines compared to Thr57. The spatial distribution is thus more comparable to the position of the known glycosylation site in the murine PSGL-1 sequence.

Figure S2. Lectin and antibody staining of the glycosulfopeptide PSGL-1 array. Related to Figure 3.

A) Microarray was probed with lectin VVA recognizing GalNAc (20 µg/mL), lectin AAL recognizing fucose (20 µg/mL), antibody to the human PSGL-1 sequence (KPL1, 5 µg/mL) and antibody to sulfotyrosine (5 µg/mL). Peptide 6 and 8 showed low signals due to the low printing efficiency of these two samples, but the remaining binding patterns confirmed the presence of the PSGL-1 peptide sequence and the modifications. B) Scan of the printed microarray. Peptides with fluorescein show clear fluorescence spots. Position 6 and 8 was not successfully printed, even after repurification and re-printing (not shown). C) Representation of the different glycoforms produced, for human and mouse PSGL-1 and for sulfated and non-sulfated peptides. For a comprehensive list, see Figure 2 and Table S1. Y-axis is average/mean relative fluorescent units (RFUs) and X-axis is glycosulfopeptide ID.

Figure S3. Chemokine binding to the microarray. Related to Figure 4.

The microarray was probed with CCL19, CCL21, and CCL5 to investigate the effect of different glycan structures and sulfation status for binding. Y-axis shows the average/mean RFU and x-axis indicates the glycosulfopeptide ID. CCL19 and CCL21 showed very similar

binding with tyrosine sulfation being pivotal for binding, whereas di-sialyl-Lex (**26**) and 2 X SLex (**27**) almost completely abolished the binding of both CCL19 and CCL21 to human PSGL-1. In the mouse sequences, less complex structures such as di-sialyl T and sialylated branch core 2 structures also blocked the CCL19 and CCL21 binding. CCL5 binding is less affected by the glycan structures, but is dependent on tyrosine sulfation and shows weaker binding to mouse PSGL-1 compared to human PSGL-1 peptides. CCL5 also shows binding to the recombinant PSGL-1. After neuraminidase treatment of the array and incubation with CCL19 there was generally lower binding, however the recombinant PSGL-1 was able to bind CCL19. We did not confirm that all sialic acids were removed.

Figure S4. Recombinant PSGL1 N-terminal O-glycosylation analysis. Related to MS/MS analysis in Star Methods.

2 µg of protein was digested and analyzed by an Orbitrap Fusion Lumos mass spectrometer to determinate the glycosylation status and revealed only glycosylation on Threonine 57 and not Threonine 44. a) HCD MS/MS spectrum of the AspN-treated O-glycopeptide $_{52}$DFLPETEPPEMLR$_{64}$ containing the O-glycan $HexNAc_2Hex_2Fuc_1$ m/z 817.3681 $[M+3H]^{3+}$. b) HCD MS/MS spectrum of the tryptic O-glycopeptide $_{44}$TEY(sulfo)EY(sulfo)LDY(sulfo)DFLPETEPPEMLR$_{64}$ containing the O-glycan $HexNAc_2Hex_2Fuc_1$ m/z 1256.1367 $[M+3H]^{3+}$.

Figure S5. Sulfonates cannot substitute tyrosine sulfates for efficient chemokine binding. Related to Figure 4.

a, b) Recombinant chemokines CCL19 and CCL21 were used to probe binding to a glycosulfopeptide array containing sulfated and sulfonated peptides. The chemokines only bound to the sulfated peptides, whereas c) PL1 antibody (Santa Cruz) recognizing the PSGL-1 N-terminal sequence bound to all peptides. d) Sequences of analyzed peptides. Y in red means tyrosine sulfate, F in red means sulfonated tyrosines.

Figure S6. Detection and purification of peptides and Enzymatic elongation of glycans and monitoring by MALDI-TOF. Related to Enzymatic Elongation and HPLC analysis and purification in Star Methods.

(A) HPLC and MALDI profiles of peptide #7 (left) and peptide #17 (right). Two peaks are observed for the released peptide 7# and the re-run of individually purified peaks due to

isomerization of 5- and 6-carboxyfluorescein. The MALDI profile of purified peptide #7 shows one single peak and no contamination. The sulfated peptide #17 shows earlier retention time but also has two peaks due to isomerization 5- and 6-carboxyfluorescein. MALDI analysis of both peaks shows identical masses corresponding to the peptide with 1 and 2 sulfates as the third sites is lost during ionization. MALDI analysis of the combined peaks shows identical masses. (B) Generation of the most complex glycan structure in the glycosulfopeptide library, a di-sialyl-Le^x. The peptide was synthesized with a core-2 O-glycan as described in materials and methods. The glycan was then sequentially elongated by addition of specific glycosyltransferases and the elongations were confirmed by MALDI-TOF.

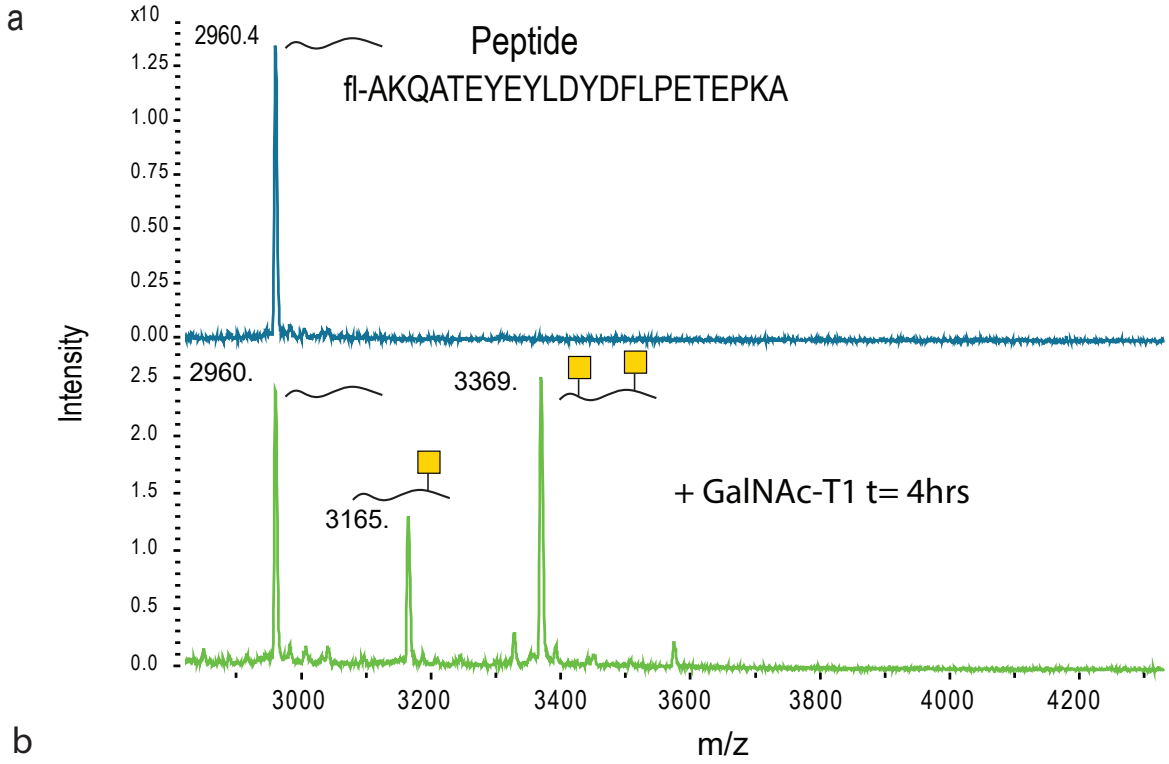
Supplementary Table Legends

Table S1. Table of all synthesized peptides. Related to Figure 2.

Peptides sequences with Id number are shown. Glycans and sulfations are shown in brackets for modified peptides. All peptides carry N-terminal fluorescein.

Table S2. Theoretical observed masses are shown for all peptides. Related to MALDI-TOF analysis of Peptides in Star Methods.

Calculated masses for sulfated PSGL-1 peptides are shown for the form with 2 sulfates (human) and 1 sulfate (murine) as these represent the major peaks in the corresponding MALDI spectra. Consistent loss of 1 sulfate was observed for the major peaks in all sulfated peptide spectra, due to in-source fragmentation. Masses were internally calibrated using calculated masses of all peptides due to the unavailability of commercial standards spanning the range of masses observed in this set of peptides for negative ionization mode. All MALDI spectra provided in Harvard Dataverse repository (DOI provided in Key Resources Table).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0.25
0.00
2960.4
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Intensity
2960.
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2.0
1.5
1.0
0.5
0.0
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3165.
+ GalNAc-T1 t= 4hrs
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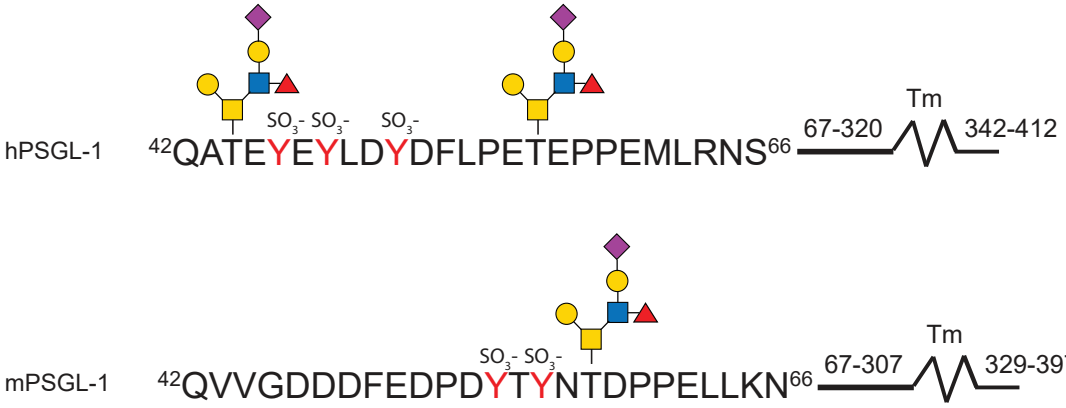
3200
3400
3600
3800
4000
4200
m/z

b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SO3-
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Tm
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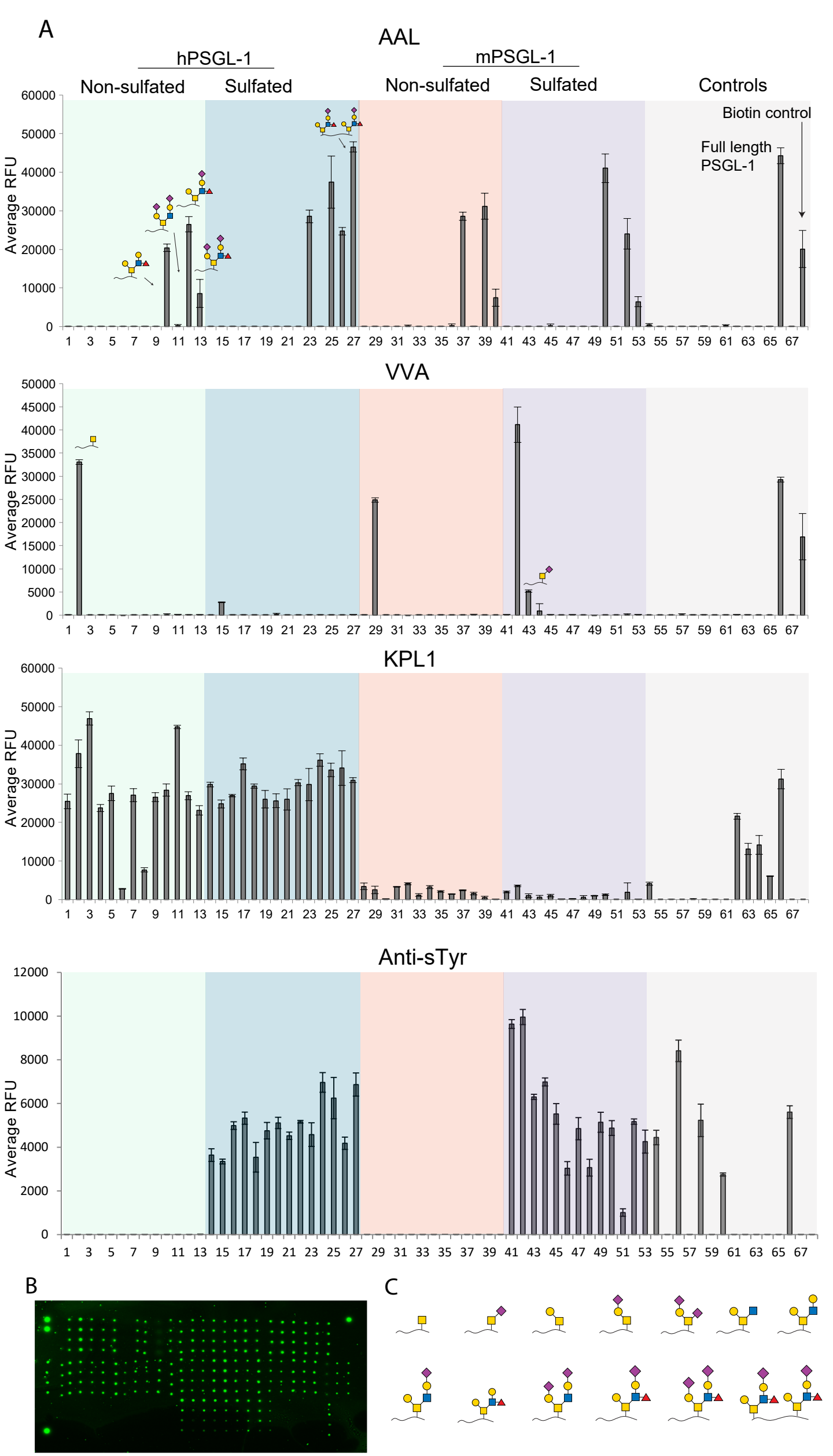
329-397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AAL
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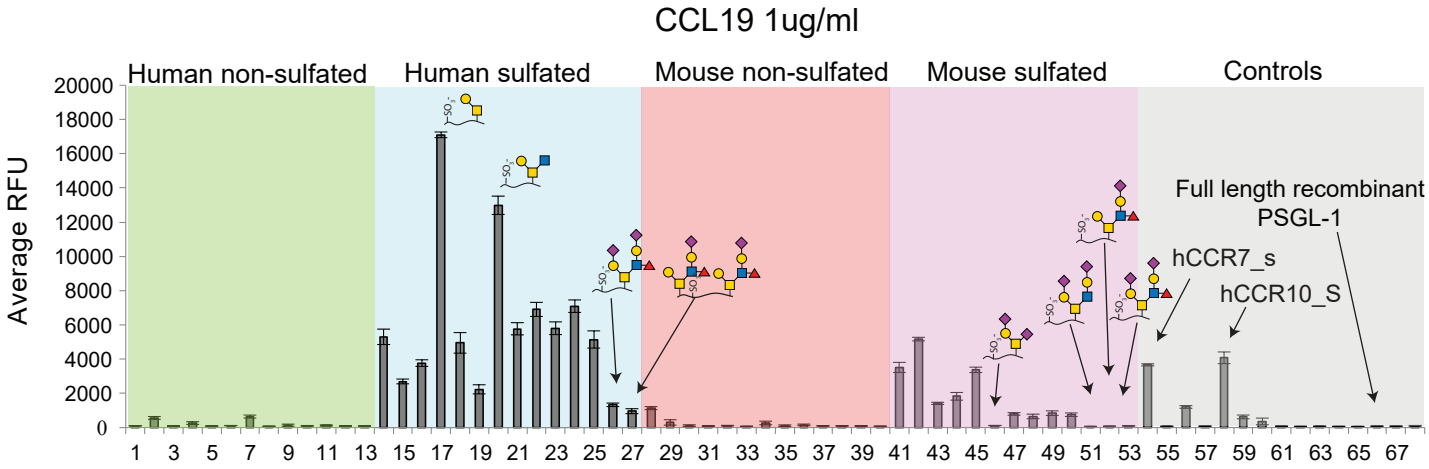
mPSGL-1
Non-sulfated
Sulfated
Non-sulfated
Sulfated
Controls
Biotin control
Full length PSGL-1
Average RFU
VVA
KPL1
Anti-sTyr
B
C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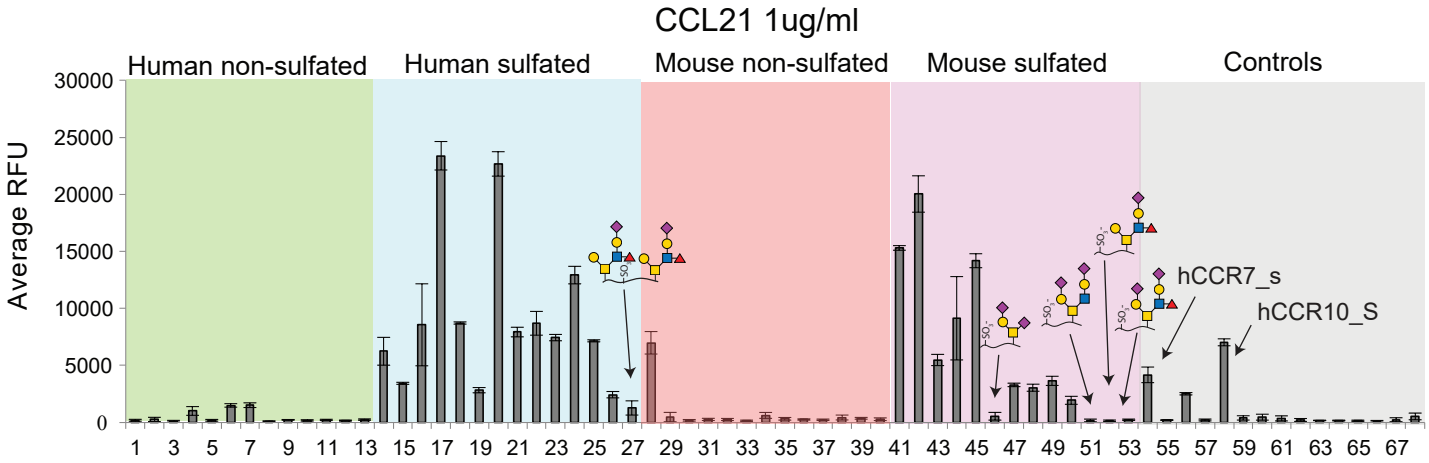
Human non-sulfated
Human sulfated
Mouse non-sulfated
Mouse sulfated
Controls
Average RFU
Full length recombinant PSGL-1
hCCR7_s
hCCR10_S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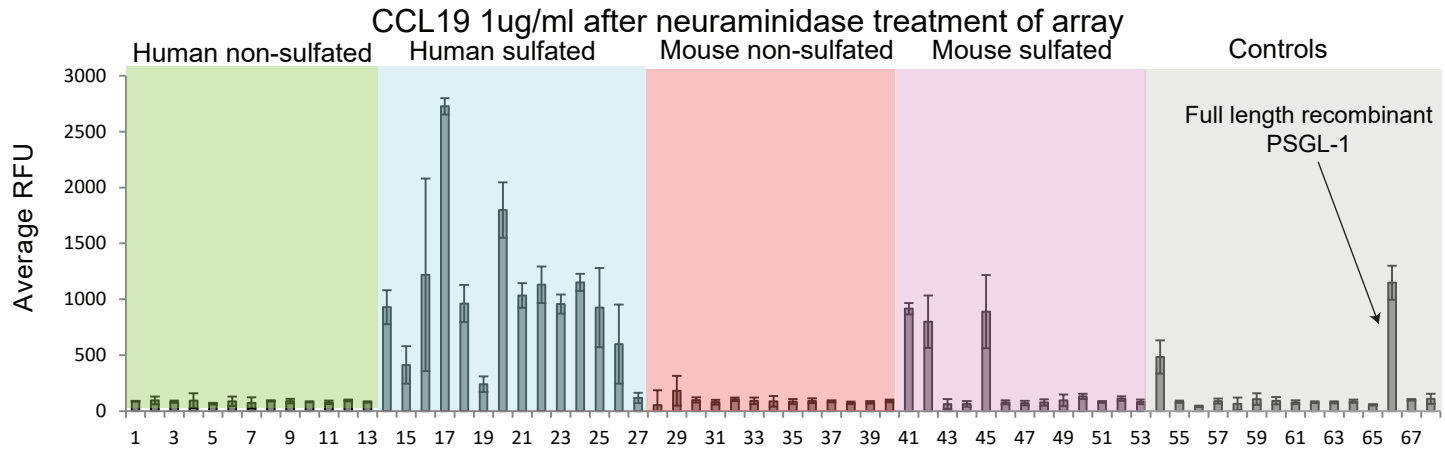
Human sulfated
Mouse non-sulfated
Mouse sulfated
Controls
Average RFU
hCCR7_s
hCCR10_S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Human sulfated
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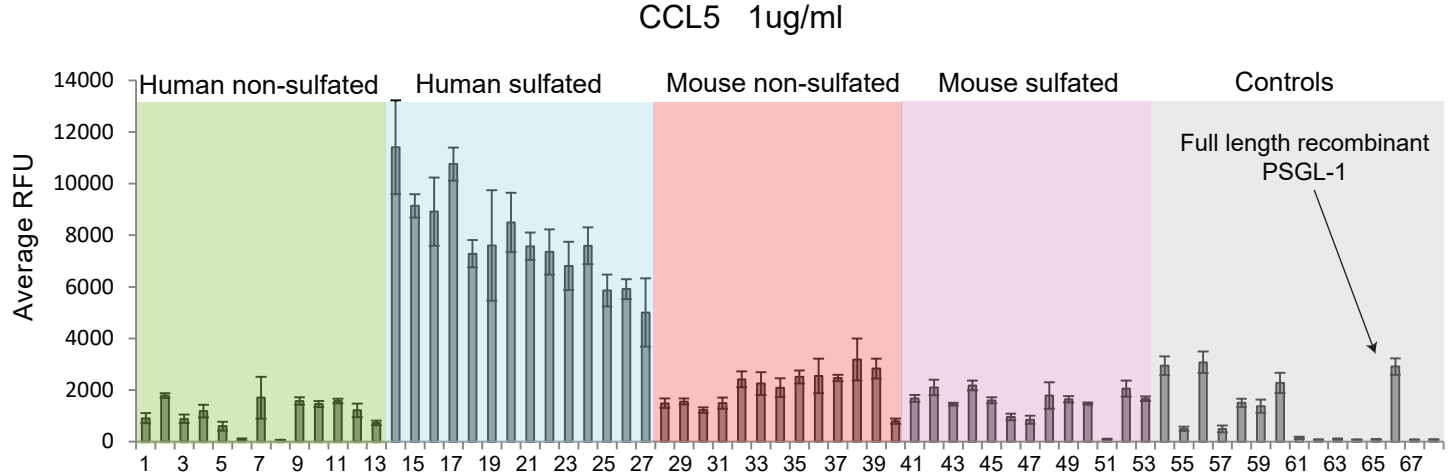
Mouse sulfated
Controls
Average RFU
Full length recombinant PSGL-1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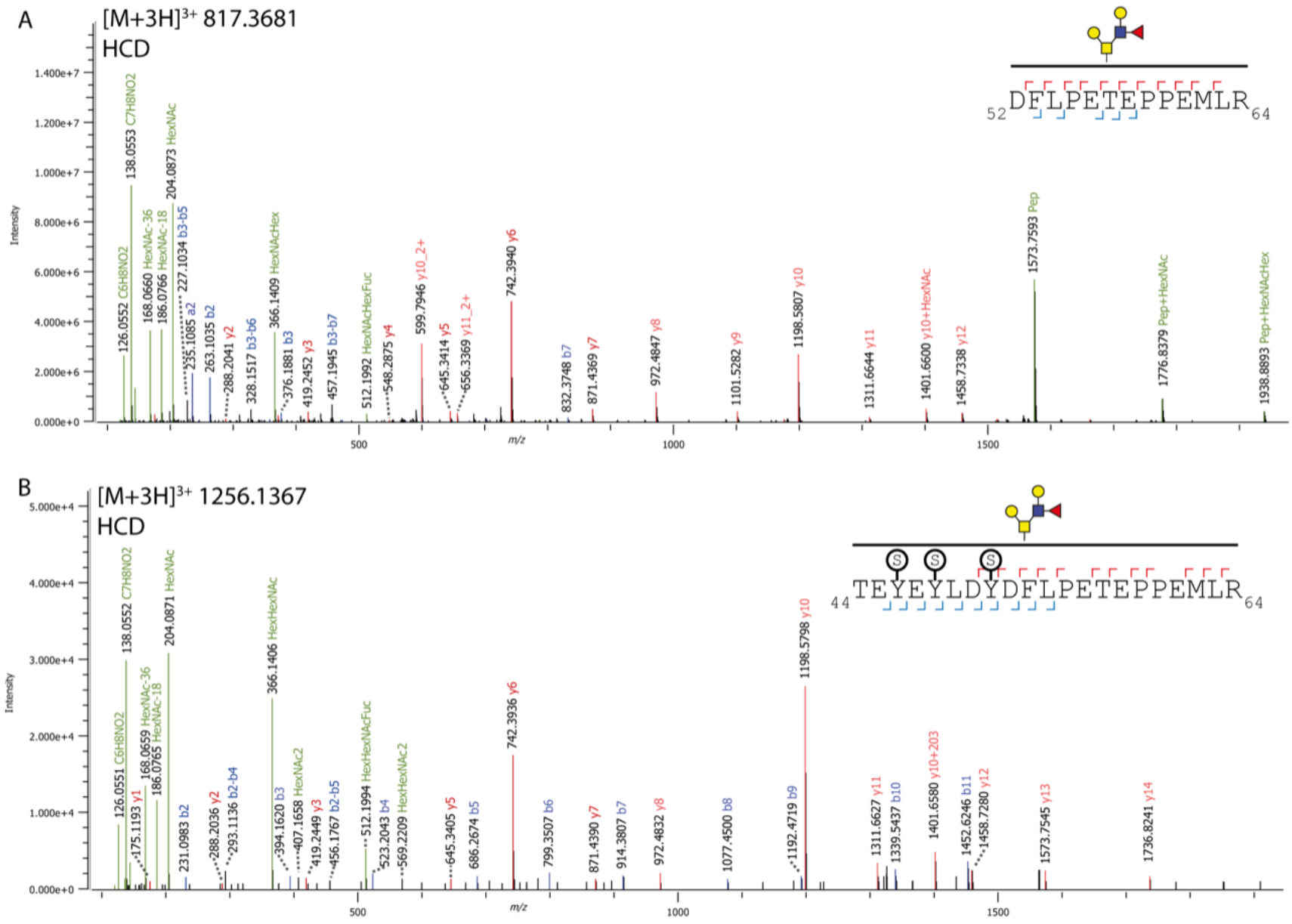
Human sulfated
Mouse non-sulfated
Mouse sulfated
Controls
Average RFU
Full length recombinant PSGL-1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Intensity
m/z
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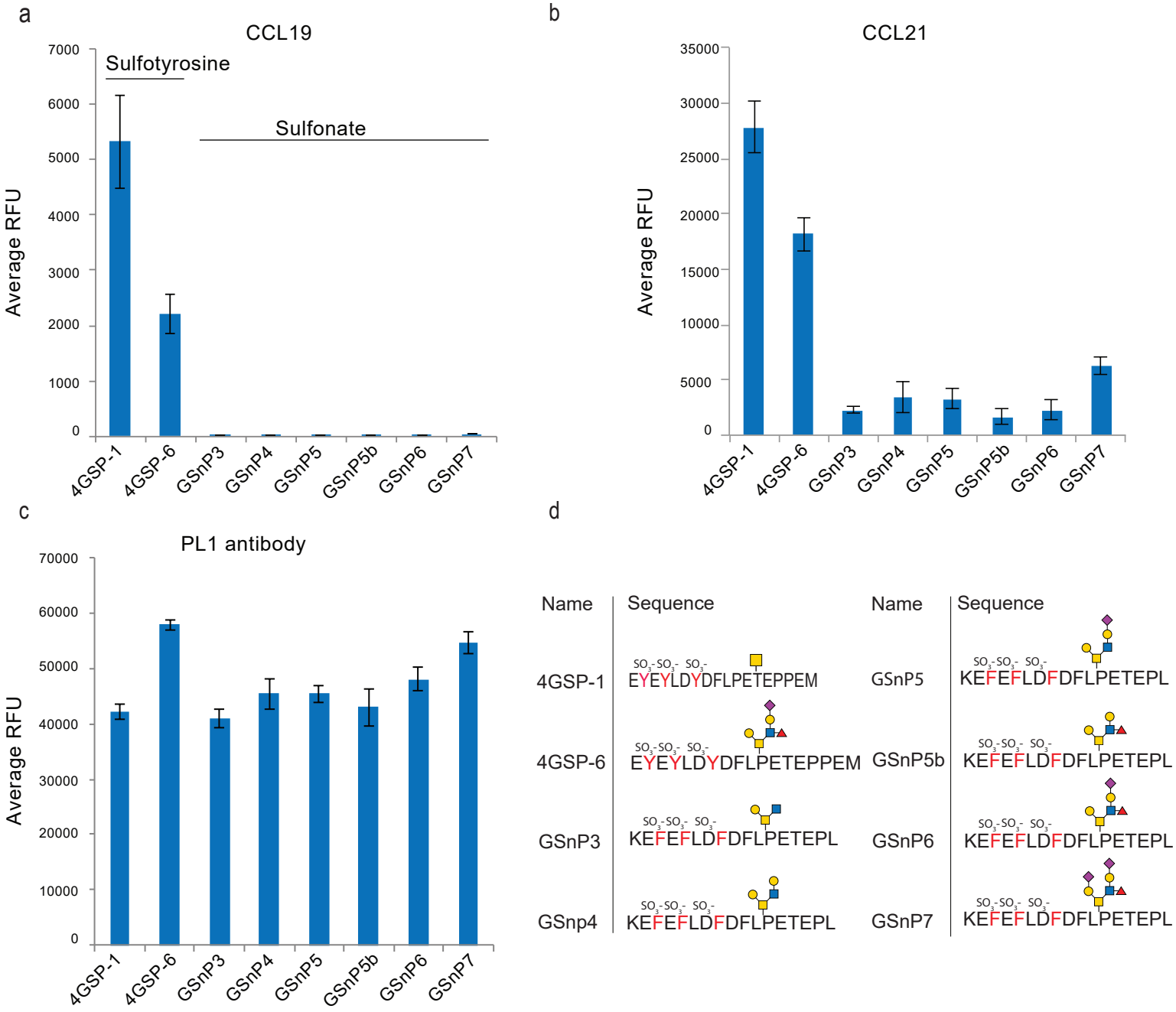
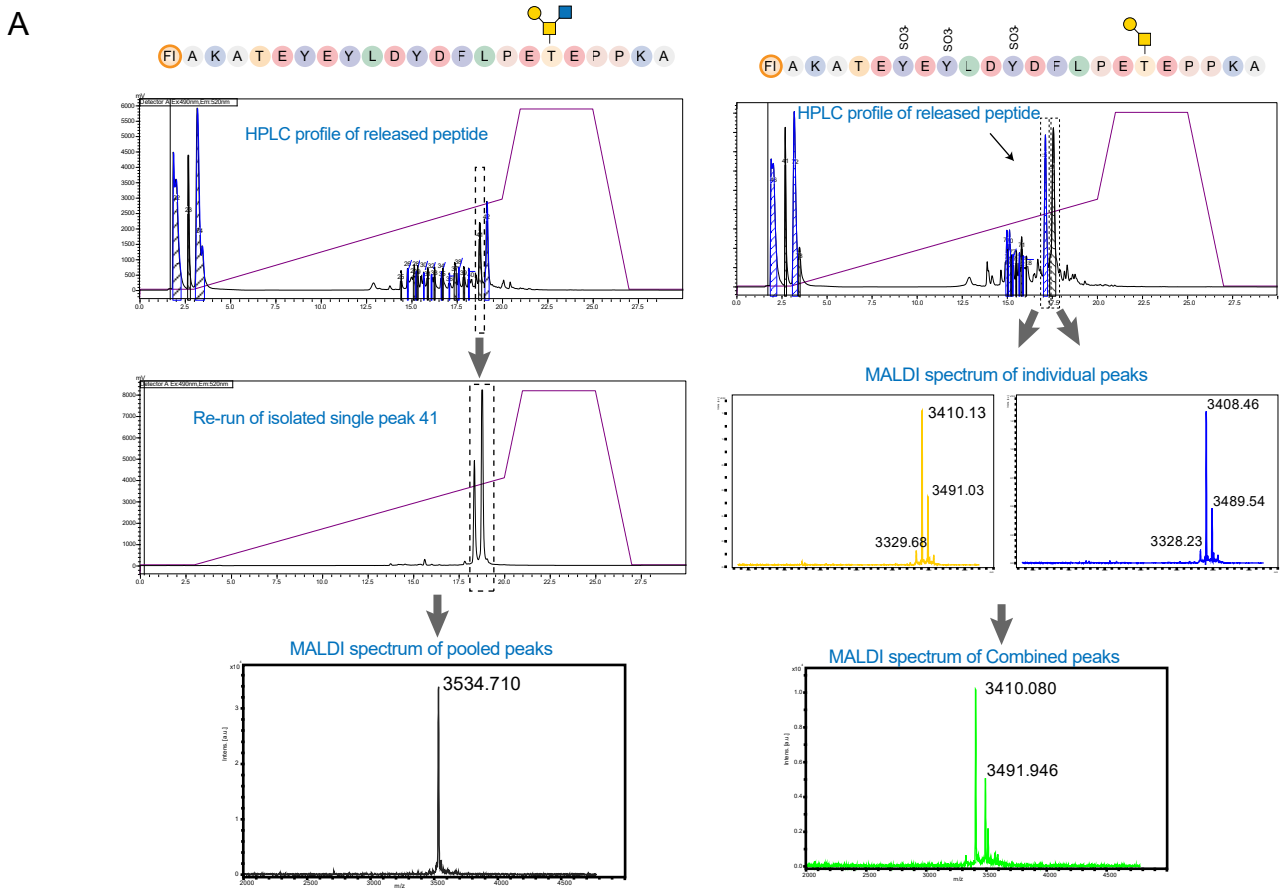
Intensity
m/z

Differences between binding of peptides with tyrosine sulfate and sulfonated tyrosine

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Re-run of isolated single peak 41
MALDI spectrum of pooled peaks
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HPLC profile of released peptide
MALDI spectrum of individual peaks
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3491.946

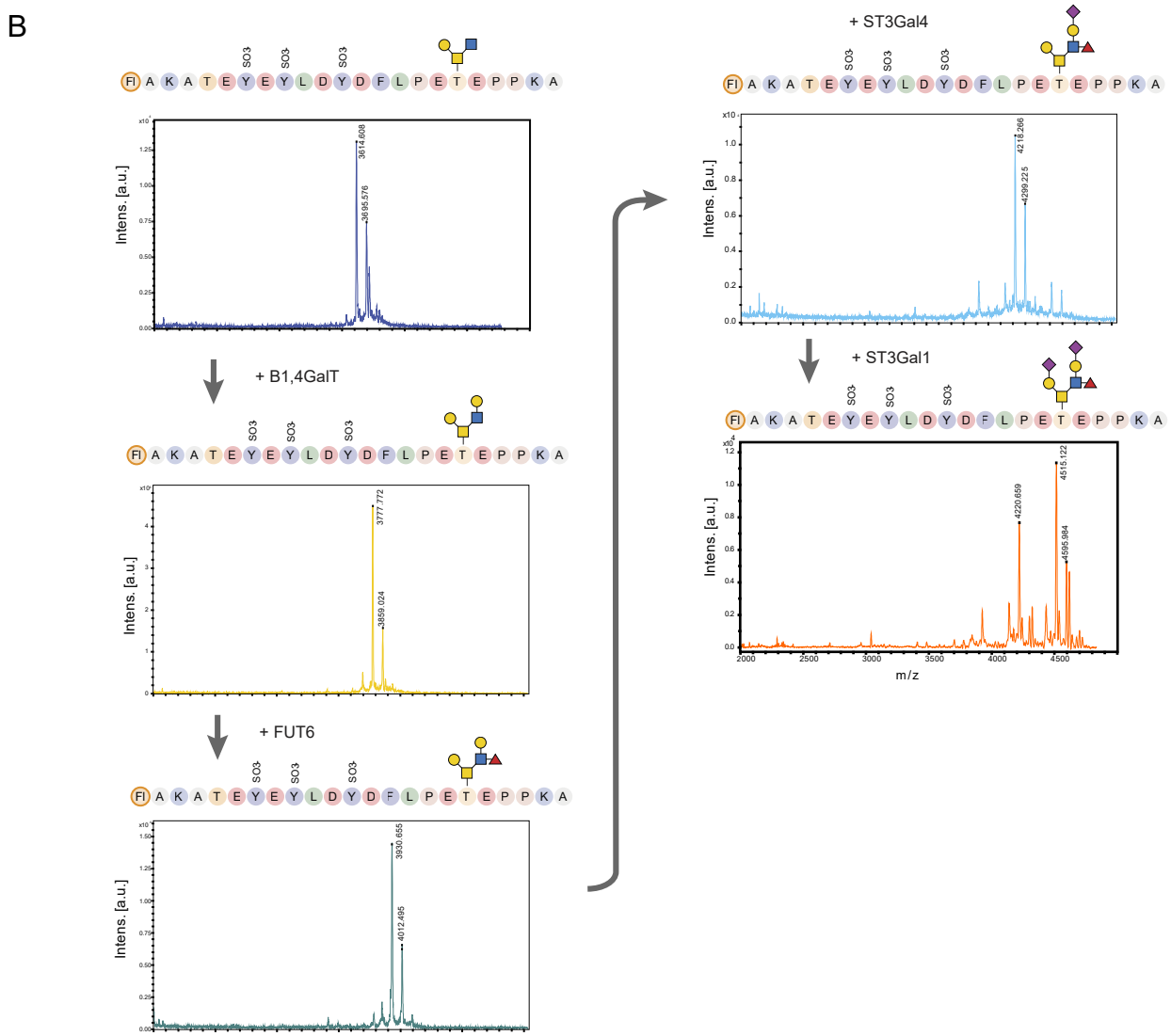
B
+ B1,4GalT
+ FUT6
+ ST3Gal4
+ ST3Gal1
Intens. [a.u.]
m/z

Table S1.

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63	4GSP1	NH2-E{sY}E{sY}LD{sY}DFLPE{GalNAca1-T}EPPEM-COOH
64	4GSP1_core2_SA	NH2-E{sY}E{sY}LD{sY}DFLPE{Neu5Aca2-3Galb1-4GlcNAca1-6(Galb1-3)GalNAca1-T}EPPEM-COOH
65	4GSP1_slex	NH2-E{sY}E{sY}LD{sY}DFLPE{Neu5Aca2-3Galb1-4(Fuca1-3)GlcNAca1-6(Galb1-3)GalNAca1-T}EPPEM-COOH
	Key	
	NH2-	N-terminus
	-COOH	C-terminus
	<5(6)-FAM>NH-	N-terminus modified with 5(6)-FAM
	-CO<OCH3>	C-terminus with O-methyl ester
	{...}	Modified amino acid (unless {sY} it is glycosylated)
	{sY}	Tyrosine Sulfate

Table S2.

Summary of calculated, observed and calibrated masses

Peptide name	ID	Theor. Mass	Obs. Mass	Calib. Obs. mass*	Nr. of sulfates
h	1	2961.287	2961.08	2962.177	-
h_GalNac	2	3164.367	3166.43	3165.313	-
h_sTn	3	3455.462	3457.46	3453.205	-
h_core1	4	3326.42	3329.5	3326.624	-
h_sT	5	3617.515	3625.66	3619.591	-
h_dsT	6	3908.611	3917.39	3908.176	-
h_core2	7	3529.499	3534.71	3529.622	-
h_core2_gal	8	3691.552	3694.48	3687.669	-
h_Core2_Gal_SA	9	3982.647	3989.89	3979.894	-
h_Core2_Gal_Fuc	10	3837.61	3845.28	3836.843	-
h_Core2_Gal_SA_SA	11	4273.743	4284.52	4271.347	-
h_sLeX	12	4128.705	4140	4128.386	-
h_dsLeX	13	4419.801	4434.84	4420.047	-
h_S	14	3121.201	3124.02	3123.360	2
h_S_GalNac	15	3324.28	3328.228	3325.367	2
h_S_sTn	16	3615.376	3622.57	3616.535	2
h_S_core1	17	3486.333	3491.95	3487.323	2
h_S_sT	18	3777.429	3785.36	3777.570	2
h_S_dsT	19	4068.524	4082.71	4071.713	2
h_S_core2	20	3689.413	3695.58	3688.758	2
h_S_core2_gal	21	3851.466	3859.02	3850.435	2
h_S_Core2_Gal_SA	22	4142.561	4152.49	4140.741	2
h_S_Core2_Gal_Fuc	23	3997.523	4012.5	4002.260	2
h_S_Core2_Gal_SA_SA	24	4433.656	4447.63	4432.699	2
h_S_sLeX	25	4288.619	4299.23	4285.899	2
h_S_dsLeX	26	4579.714	4595.98	4579.449	2
h_S_ 2X sLeX	27	5456.037	5486.33	5460.199	2
m	28	2844.132	2844.37	2846.726	-
m_GalNAc	29	3047.211	3048.44	3048.595	-
m__sTn	30	3338.307	3338.87	3335.894	-
m_Core1	31	3209.264	3209.92	3208.334	-
m_sT	32	3500.359	3505.7	3500.925	-
m_dsT	33	3791.455	3795.98	3788.075	-
m_core-2	34	3412.343	3415.18	3411.381	-
m_core-2_Gal	35	3574.396	3577.4	3571.852	-
m_core-2_SA	36	3703.439	3708.6	3701.637	-
m_Core2_Gal_Fuc	37	3720.454	3725.68	3718.533	-
m_Core2_Gal_SA_SA	38	4156.587	4167.86	4155.945	-
m_sLeX	39	4011.549	4022.55	4012.202	-
m_dsLeX	40	4302.645	4320.05	4306.494	-
m_S	41	2924.089	2920.45	2921.985	1
m_S_GalNAc	42	3127.168	3129.35	3128.633	1
m_S_sTn	43	3418.263	3422.72	3418.840	1
m_S_Core1	44	3289.221	3292.29	3289.816	1
m_S_sT	45	3580.316	3586.83	3581.180	1
m_S_dsT	46	3871.412	3880.79	3871.971	1

m_S_Core-2	47	3492.3	3497.4	3492.714	1
m_S_core-2_Gal	48	3654.353	3658.68	3652.255	1
m_S_core-2_SA	49	3783.396	3788.93	3781.101	1
m_S_Core2_Gal_Fuc	50	3800.411	3808.27	3800.233	1
m_S_Core2_Gal_SA_SA	51	4236.544	4249.33	4236.537	1
m_S_sLeX	52	4091.506	4103.7	4092.477	1
m_S_dsLeX	53	4382.602	4398.09	4383.693	1
CCR7_hum_sulf	54	2930.208	2932.17	2933.579	2
CCR7_hum	55	2850.251	2847.49	2849.812	-
CCR7_mouse_sulf	56	3026.16	3025.86	3026.259	-
CCR7_mouse	57	2866.246	2865.02	2867.153	1
CCR10_hum_sulf	58	2815.083	2812.42	2815.120	-
CCR10_hum	59	2735.127	2731.67	2735.241	-
CCR10_mouse_sulf	60	2875.112	2871.48	2873.543	2
CCR10_mouse	61	2715.198	2712.7	2716.475	-