Supplementary Information for

A systematic assessment of structural heterogeneity and IgG/IgE-binding of ovalbumin

Wenhua Yang, ✉ Zongcai Tu, ✉ David Julian McClements and Igor A. Kaltashov

Contents

Table S1. Information about HEA patients.

No.	Gender	Age (year)	Clinical symptoms	Other allergens	IgE (kU L^{-1})
1	Male	5	AS, EC	Milk	15.4
2	Male	16	AS, HI	Peanut, Soybean	13.7
3	Female	51	EC, RH	Walnut, Cottonwood	11.5
4	Male	27	HI, NW	Most food allergy	29.8
5	Male	28	AS, HI	Peanut, Soybean	21.3
6	Female	47	HI, CW	Most food allergy	64.6
7	Male	49	AS, NW	Codfish, Wheat	24.2
8	Male	33	EC, RH	Wheat, Shrimp	10.8

AS, asthma; HI, hives; EC, eczema; RH, rhinitis; NW, nose wheezing; CW, chest wheezing

Table S2. Analysis of ovalbumin species.

No.	ID	Modification				Glycan in N292			Exp. Mass Da	Theor. Mass Da	Δm Da	Ratio %	
		A	P	S	O	Hex	GlcNAc	NeuAc					
1	**P1-1(1-0-0-0-8-7-0)**	**1**	**0**	**0**	**0**	**8**	**7**	**0**	**45507.6**	**45509.2**	**-1.6**	**0.03**	*
2	P1-2(1-0-0-0-9-7-0)	1	0	0	0	9	7	0	45669.6	45671.3	-1.7	0.03	*
3	P1-3(1-0-0-0-8-8-0)	1	0	0	0	8	8	0	45711.4	45712.4	-1.0	0.06	*
4	P1-4(1-0-0-0-9-8-0)	1	0	0	0	9	8	0	45871.9	45874.3	-2.4	0.08	*
5	P1-5(1-0-0-0-8-9-0)	1	0	0	0	8	9	0	45916.8	45915.6	1.2	0.03	*
6	P1-6(1-0-0-0-10-8-0)	1	0	0	0	10	8	0	46036.8	46036.7	0.1	0.04	*
7	P1-7(1-0-0-0-8-10-0)	1	0	0	0	8	10	0	46118.4	46118.8	-0.4	0.05	*
8	P1-8(1-0-0-0-8-11-0)	1	0	0	0	8	11	0	46320.0	46322.0	-2.0	0.03	*
9	P1-9(1-0-0-0-9-11-0)	1	0	0	0	9	11	0	46480.8	46484.1	-3.3	0.02	*
10	P2-1(1-0-0-0-5-2-0)	1	0	0	0	5	2	0	44005.4	44006.8	-1.4	0.12	
11	P2-2(1-0-0-0-6-2-0)	1	0	0	0	6	2	0	44167.2	44168.9	-1.7	0.19	
12	P2-3(1-0-0-0-7-2-0)	1	0	0	0	7	2	0	44328.0	44331.1	-3.1	0.05	
13	P2-4(1-0-0-0-5-4-0)	1	0	0	0	5	4	0	44412.0	44413.2	-1.2	0.12	
14	P2-5(1-0-0-0-5-5-0)	1	0	0	0	5	5	0	44616.0	44616.4	-0.4	0.03	*
15	P2-6(1-0-0-0-6-5-0)	1	0	0	0	6	5	0	44778.0	44778.5	-0.5	0.02	*
16	P3-1(1-1-1-0-5-2-0)	1	1	1	0	5	2	0	44066.4	44068.8	-2.4	0.11	*
17	P3-2(1-1-1-0-6-2-0)	1	1	1	0	6	2	0	44227.2	44230.9	-3.7	0.17	*
18	P3-3(1-1-1-0-7-2-0)	1	1	1	0	7	2	0	44390.4	44393.1	-2.7	0.06	*
19	P3-4(1-1-1-0-5-4-0)	1	1	1	0	5	4	0	44473.2	44475.2	-2.0	0.12	*
20	P3-5(1-1-1-0-5-5-0)	1	1	1	0	5	5	0	44677.2	44678.4	-1.2	0.04	*
21	**P3-6(1-1-0-0-8-7-0)**	**1**	**1**	**0**	**0**	**8**	**7**	**0**	**45589.2**	**45589.2**	**0.0**	**0.03**	
22	**P3-7(1-1-0-0-9-7-0)**	**1**	**1**	**0**	**0**	**9**	**7**	**0**	**45752.4**	**45751.3**	**1.1**	**0.05**	*
23	**P3-8(1-1-0-0-8-8-0)**	**1**	**1**	**0**	**0**	**8**	**8**	**0**	**45793.2**	**45792.4**	**0.8**	**0.12**	*
24	**P3-9(1-1-0-0-9-8-0)**	**1**	**1**	**0**	**0**	**9**	**8**	**0**	**45952.8**	**45954.5**	**-1.7**	**0.18**	*
25	**P3-10(1-1-0-0-8-9-0)**	**1**	**1**	**0**	**0**	**8**	**9**	**0**	**45996.0**	**45995.6**	**0.4**	**0.05**	*
26	**P3-11(1-1-0-0-10-8-0)**	**1**	**1**	**0**	**0**	**10**	**8**	**0**	**46113.6**	**46116.6**	**-3.0**	**0.09**	*
27	**P3-12(1-1-0-0-8-10-0)**	**1**	**1**	**0**	**0**	**8**	**10**	**0**	**46196.4**	**46198.8**	**-2.4**	**0.11**	*
28	**P3-13(1-1-0-0-7-11-0)**	**1**	**1**	**0**	**0**	**7**	**11**	**0**	**46236.0**	**46239.8**	**-3.8**	**0.04**	*
29	**P3-14(1-1-0-0-9-10-0)**	**1**	**1**	**0**	**0**	**9**	**10**	**0**	**46359.8**	**46360.9**	**-1.1**	**0.05**	*
30	**P3-15(1-1-0-0-8-11-0)**	**1**	**1**	**0**	**0**	**8**	**11**	**0**	**46400.4**	**46401.9**	**-1.5**	**0.06**	*
31	**P3-16(1-1-0-0-9-11-0)**	**1**	**1**	**0**	**0**	**9**	**11**	**0**	**46561.2**	**46564.1**	**-2.9**	**0.04**	*
32	P4-1(0-1-0-0-5-2-0)	0	1	0	0	5	2	0	44042.4	44044.8	-2.4	0.11	*
33	P4-2(0-1-0-0-6-2-0)	0	1	0	0	6	2	0	44204.4	44206.9	-2.5	0.23	
34	P4-3(0-1-0-0-7-2-0)	0	1	0	0	7	2	0	44365.2	44369.0	-3.8	0.06	*
35	P4-4(0-1-0-0-5-4-0)	0	1	0	0	5	4	0	44449.2	44451.1	-1.9	0.13	

Table S2. continued

No.	ID	Modification				Glycan in N292			Exp. Mass Da	Theor. Mass Da	Δm Da	Ratio %	
		A	P	S	O	Hex	GlcNAc	NeuAc					
36	P4-5(0-1-0-0-5-5-0)	0	1	0	0	5	5	0	44653.2	44654.3	-1.1	0.04	*
37	P4-6(0-1-0-0-6-5-0)	0	1	0	0	6	5	0	44815.2	44816.5	-1.3	0.02	*
38	P5-1(1-1-0-0-4-2-0)	1	1	0	0	4	2	0	43922.4	43924.6	-2.2	0.08	
39	**P5-2(1-1-0-0-5-2-0)**	**1**	**1**	**0**	**0**	**5**	**2**	**0**	**44084.4**	**44086.8**	**-2.4**	**2.21**	
40	**P5-3(1-1-0-0-6-2-0)**	**1**	**1**	**0**	**0**	**6**	**2**	**0**	**44247.6**	**44248.9**	**-1.3**	**3.41**	
41	**P5-4(1-1-0-0-5-3-0)**	**1**	**1**	**0**	**0**	**5**	**3**	**0**	**44292.0**	**44290.0**	**2.0**	**0.36**	
42	**P5-5(1-1-0-0-4-4-0)**	**1**	**1**	**0**	**0**	**4**	**4**	**0**	**44330.4**	**44331.0**	**-0.6**	**0.22**	
43	**P5-6(1-1-0-0-7-2-0)**	**1**	**1**	**0**	**0**	**7**	**2**	**0**	**44409.6**	**44411.1**	**-1.5**	**0.94**	
44	**P5-7(1-1-0-0-5-4-0)**	**1**	**1**	**0**	**0**	**5**	**4**	**0**	**44492.4**	**44493.2**	**-0.8**	**1.95**	
45	**P5-8(1-1-0-0-4-5-0)**	**1**	**1**	**0**	**0**	**4**	**5**	**0**	**44534.4**	**44534.2**	**0.2**	**0.24**	
46	**P5-9(1-1-0-0-3-6-0)**	**1**	**1**	**0**	**0**	**3**	**6**	**0**	**44575.2**	**44575.3**	**-0.1**	**0.12**	
47	**P5-10(1-1-0-0-5-5-0)**	**1**	**1**	**0**	**0**	**5**	**5**	**0**	**44694.0**	**44696.4**	**-2.4**	**0.44**	
48	**P5-11(1-1-0-0-4-6-0)**	**1**	**1**	**0**	**0**	**4**	**6**	**0**	**44738.4**	**44737.4**	**1.0**	**0.06**	*
49	**P5-12(1-1-0-0-6-5-0)**	**1**	**1**	**0**	**0**	**6**	**5**	**0**	**44857.2**	**44858.5**	**-1.3**	**0.20**	*
50	P5-13(1-1-0-0-5-6-0)	1	1	0	0	5	6	0	44901.6	44899.6	2.0	0.02	*
51	P5-14(1-1-0-0-7-5-0)	1	1	0	0	7	5	0	45018.0	45020.6	-2.6	0.01	*
52	**P6-1(1-1-0-0-8-7-0)**	**1**	**1**	**0**	**0**	**8**	**7**	**0**	**45586.8**	**45589.2**	**-2.4**	**0.01**	
53	**P6-2(1-1-0-0-9-7-0)**	**1**	**1**	**0**	**0**	**9**	**7**	**0**	**45747.6**	**45751.3**	**-3.7**	**0.02**	*
54	**P6-3(1-1-0-0-8-8-0)**	**1**	**1**	**0**	**0**	**8**	**8**	**0**	**45789.6**	**45792.4**	**-2.8**	**0.06**	*
55	**P6-4(1-1-0-0-9-8-0)**	**1**	**1**	**0**	**0**	**9**	**8**	**0**	**45952.8**	**45954.5**	**-1.7**	**0.15**	*
56	**P6-5(1-1-0-0-8-9-0)**	**1**	**1**	**0**	**0**	**8**	**9**	**0**	**45996.0**	**45995.6**	**0.4**	**0.03**	*
57	**P6-6(1-1-0-0-10-8-0)**	**1**	**1**	**0**	**0**	**10**	**8**	**0**	**46113.6**	**46116.6**	**-3.0**	**0.06**	*
58	**P6-7(1-1-0-0-8-10-0)**	**1**	**1**	**0**	**0**	**8**	**10**	**0**	**46196.4**	**46198.8**	**-2.4**	**0.06**	*
59	**P6-8(1-1-0-0-7-11-0)**	**1**	**1**	**0**	**0**	**7**	**11**	**0**	**46239.6**	**46239.8**	**-0.2**	**0.02**	*
60	**P6-9(1-1-0-0-9-10-0)**	**1**	**1**	**0**	**0**	**9**	**10**	**0**	**46359.6**	**46360.9**	**-1.3**	**0.03**	*
61	**P6-10(1-1-0-0-8-11-0)**	**1**	**1**	**0**	**0**	**8**	**11**	**0**	**46400.4**	**46401.9**	**-1.5**	**0.03**	*
62	**P6-11(1-1-0-0-9-11-0)**	**1**	**1**	**0**	**0**	**9**	**11**	**0**	**46562.4**	**46564.1**	**-1.7**	**0.02**	
63	**P7-1(1-1-0-0-5-2-0)**	**1**	**1**	**0**	**0**	**5**	**2**	**0**	**44084.4**	**44086.8**	**-2.4**	**0.59**	
64	**P7-2(1-1-0-0-6-2-0)**	**1**	**1**	**0**	**0**	**6**	**2**	**0**	**44247.6**	**44248.9**	**-1.3**	**1.10**	
65	**P7-3(1-1-0-0-5-3-0)**	**1**	**1**	**0**	**0**	**5**	**3**	**0**	**44292.0**	**44290.0**	**2.0**	**0.16**	
66	**P7-4(1-1-0-0-4-4-0)**	**1**	**1**	**0**	**0**	**4**	**4**	**0**	**44330.4**	**44331.0**	**-0.6**	**0.09**	
67	**P7-5(1-1-0-0-7-2-0)**	**1**	**1**	**0**	**0**	**7**	**2**	**0**	**44409.1**	**44411.1**	**-2.0**	**0.36**	
68	**P7-6(1-1-0-0-5-4-0)**	**1**	**1**	**0**	**0**	**5**	**4**	**0**	**44492.4**	**44493.2**	**-0.8**	**0.58**	
69	**P7-7(1-1-0-0-4-5-0)**	**1**	**1**	**0**	**0**	**4**	**5**	**0**	**44534.4**	**44534.2**	**0.2**	**0.13**	
70	**P7-8(1-1-0-0-3-6-0)**	**1**	**1**	**0**	**0**	**3**	**6**	**0**	**44575.2**	**44575.3**	**-0.1**	**0.07**	

Table S2. continued

No.	ID	Modification				Glycan in N292			Exp. Mass Da	Theor. Mass Da	Δm Da	Ratio %	
		A	P	S	O	Hex	GlcNAc	NeuAc					
71	**P7-9(1-1-0-0-5-5-0)**	**1**	**1**	**0**	**0**	**5**	**5**	**0**	**44695.2**	**44696.4**	**-1.2**	**0.15**	
72	**P7-10(1-1-0-0-4-6-0)**	**1**	**1**	**0**	**0**	**4**	**6**	**0**	**44738.4**	**44737.4**	**1.0**	**0.03**	*
73	**P7-11(1-1-0-0-6-5-0)**	**1**	**1**	**0**	**0**	**6**	**5**	**0**	**44857.2**	**44858.5**	**-1.3**	**0.06**	*
74	P7-12(1-1-0-0-3-2-1)	1	1	0	0	3	2	1	44056.8	44053.8	3.0	0.12	*
75	P7-13(1-1-0-0-4-2-1)	1	1	0	0	4	2	1	44218.8	44215.9	2.9	0.23	*
76	P7-14(1-1-0-0-5-2-1)	1	1	0	0	5	2	1	44380.8	44378.0	2.8	0.09	*
77	P7-15(1-1-0-0-3-4-1)	1	1	0	0	3	4	1	44461.2	44460.1	1.1	0.16	*
78	P7-16(1-1-0-0-5-5-1)	1	1	0	0	5	5	1	44985.6	44987.6	-2.0	0.04	*
79	P7-17(1-1-0-0-4-6-1)	1	1	0	0	4	6	1	45028.8	45028.7	0.1	0.02	*
80	P7-18(1-1-0-0-6-5-1)	1	1	0	0	6	5	1	45147.6	45149.8	-2.2	0.03	*
81	P8-1(1-2-1-0-5-2-0)	1	2	1	0	5	2	0	44146.8	44148.8	-2.0	0.41	
82	P8-2(1-2-1-0-6-2-0)	1	2	1	0	6	2	0	44308.8	44310.9	-2.1	0.90	
83	P8-3(1-2-1-0-7-2-0)	1	2	1	0	7	2	0	44470.8	44473.0	-2.2	0.31	*
84	P8-4(1-2-1-0-5-4-0)	1	2	1	0	5	4	0	44552.4	44555.2	-2.8	0.48	
85	P8-5(1-2-1-0-5-5-0)	1	2	1	0	5	5	0	44756.4	44758.3	-1.9	0.16	
86	P8-6(1-2-1-0-6-5-0)	1	2	1	0	6	5	0	44918.4	44920.5	-2.1	0.08	*
87	P8-7(1-2-0-0-8-7-0)	1	2	0	0	8	7	0	45668.4	45669.2	-0.8	0.08	
88	P8-8(1-2-0-0-9-7-0)	1	2	0	0	9	7	0	45828.0	45831.3	-3.3	0.16	
89	P8-9(1-2-0-0-8-8-0)	1	2	0	0	8	8	0	45870.0	45872.3	-2.3	0.31	
90	P8-10(1-2-0-0-9-8-0)	1	2	0	0	9	8	0	46032.0	46034.5	-2.5	0.57	*
91	P8-11(1-2-0-0-8-9-0)	1	2	0	0	8	9	0	46076.4	46075.5	0.9	0.14	*
92	P8-12(1-2-0-0-10-8-0)	1	2	0	0	10	8	0	46195.2	46196.6	-1.4	0.23	*
93	P8-13(1-2-0-0-8-10-0)	1	2	0	0	8	10	0	46276.8	46278.7	-1.9	0.27	*
94	P8-14(1-2-0-0-7-11-0)	1	2	0	0	7	11	0	46320.0	46319.8	0.2	0.09	*
95	P8-15(1-2-0-0-9-10-0)	1	2	0	0	9	10	0	46437.6	46440.9	-3.3	0.09	*
96	P8-16(1-2-0-0-8-11-0)	1	2	0	0	8	11	0	46479.6	46481.9	-2.3	0.14	*
97	P8-17(1-2-0-0-7-12-0)	1	2	0	0	7	12	0	46524.0	46523.0	1.0	0.03	*
98	P8-18(1-2-0-0-9-11-0)	1	2	0	0	9	11	0	46642.8	46644.1	-1.3	0.07	*
99	**P9-1(1-2-0-0-4-2-0)**	**1**	**2**	**0**	**0**	**4**	**2**	**0**	**44002.8**	**44004.6**	**-1.8**	**0.47**	
100	P9-2(0-2-0-0-5-2-0)	0	2	0	0	5	2	0	44122.4	44124.7	-2.3	0.50	
101	**P9-3(1-2-0-0-5-2-0)**	**1**	**2**	**0**	**0**	**5**	**2**	**0**	**44164.8**	**44166.8**	**-2.0**	**13.91**	
102	P9-4(0-2-0-0-6-2-0)	0	2	0	0	6	2	0	44284.8	44286.9	-2.1	0.84	
103	**P9-5(1-2-0-0-6-2-0)**	**1**	**2**	**0**	**0**	**6**	**2**	**0**	**44327.3**	**44328.9**	**-1.6**	**24.96**	
104	**P9-6(1-2-0-0-7-2-0)**	**1**	**2**	**0**	**0**	**7**	**2**	**0**	**44488.8**	**44491.0**	**-2.2**	**6.50**	
105	P9-7(0-2-0-0-5-4-0)	0	2	0	0	5	4	0	44529.6	44531.1	-1.5	0.86	

Table S2. continued

No.	ID	Modification				Glycan in N292			Exp. Mass Da	Theor. Mass Da	Δm Da	Ratio %	
		A	P	S	O	Hex	GlcNAc	NeuAc					
106	P9-8(1-2-0-0-5-4-0)	1	2	0	0	5	4	0	44571.6	44573.2	-1.6	12.29	
107	**P9-9(1-2-0-0-4-5-0)**	**1**	**2**	**0**	**0**	**4**	**5**	**0**	**44613.6**	**44614.2**	**-0.6**	**1.64**	
108	P9-10(1-2-0-0-3-6-0)	1	2	0	0	3	6	0	44653.2	44655.3	-2.1	0.68	
109	P9-11(1-2-0-0-6-4-0)	1	2	0	0	6	4	0	44732.4	44735.3	-2.9	1.09	
110	**P9-12(1-2-0-0-5-5-0)**	**1**	**2**	**0**	**0**	**5**	**5**	**0**	**44774.4**	**44776.3**	**-1.9**	**2.69**	
111	**P9-13(1-2-0-0-4-6-0)**	**1**	**2**	**0**	**0**	**4**	**6**	**0**	**44818.8**	**44817.4**	**1.4**	**0.37**	*
112	**P9-14(1-2-0-0-6-5-0)**	**1**	**2**	**0**	**0**	**6**	**5**	**0**	**44936.4**	**44938.5**	**-2.1**	**1.19**	
113	P9-15(1-2-0-0-7-5-0)	1	2	0	0	7	5	0	45099.1	45100.6	-1.5	0.10	*
114	**P10-1(1-2-0-0-0-0-0)**	**1**	**2**	**0**	**0**	**0**	**0**	**0**	**42948.0**	**42949.7**	**-1.7**	**0.22**	*
115	P10-2(1-2-0-0-2-4-1)	1	2	0	0	2	4	1	44374.8	44378.0	-3.2	0.08	*
116	P10-2(1-2-0-0-5-2-1)	1	2	0	0	5	2	1	44457.6	44458.0	-0.4	0.16	*
117	P10-3(1-2-0-0-6-2-1)	1	2	0	0	6	2	1	44617.2	44620.2	-3.0	0.38	*
118	P10-4(1-2-0-0-5-3-1)	1	2	0	0	5	3	1	44658.0	44661.2	-3.2	0.11	
119	P10-5(1-2-0-0-6-3-1)	1	2	0	0	6	3	1	44822.4	44823.4	-1.0	0.10	
120	**P10-6(1-2-0-0-5-5-1)**	**1**	**2**	**0**	**0**	**5**	**5**	**1**	**45066.0**	**45067.6**	**-1.6**	**0.15**	
121	P10-7(1-2-0-0-4-6-1)	1	2	0	0	4	6	1	45108.0	45108.7	-0.7	0.06	*
122	P10-8(1-2-0-0-6-5-1)	1	2	0	0	6	5	1	45228.0	45229.7	-1.7	0.10	
123	**P11-1(1-2-0-0-0-0-0)**	**1**	**2**	**0**	**0**	**0**	**0**	**0**	**42948.0**	**42949.7**	**-1.7**	**0.03**	*
124	**P11-2(1-2-0-0-4-2-0)**	**1**	**2**	**0**	**0**	**4**	**2**	**0**	**44002.8**	**44004.6**	**-1.8**	**0.02**	
125	**P11-3(1-2-0-0-5-2-0)**	**1**	**2**	**0**	**0**	**5**	**2**	**0**	**44164.8**	**44166.8**	**-2.0**	**0.84**	
126	**P11-4(1-2-0-0-6-2-0)**	**1**	**2**	**0**	**0**	**6**	**2**	**0**	**44326.8**	**44328.9**	**-2.1**	**1.80**	
127	**P11-5(1-2-0-0-7-2-0)**	**1**	**2**	**0**	**0**	**7**	**2**	**0**	**44488.8**	**44491.0**	**-2.2**	**0.56**	
128	**P11-6(1-2-0-0-5-4-0)**	**1**	**2**	**0**	**0**	**5**	**4**	**0**	**44571.6**	**44573.2**	**-1.6**	**0.94**	
129	**P11-7(1-2-0-0-4-5-0)**	**1**	**2**	**0**	**0**	**4**	**5**	**0**	**44613.6**	**44614.2**	**-0.6**	**0.22**	
130	**P11-8(1-2-0-0-5-5-0)**	**1**	**2**	**0**	**0**	**5**	**5**	**0**	**44774.4**	**44776.3**	**-1.9**	**0.27**	
131	**P11-9(1-2-0-0-4-6-0)**	**1**	**2**	**0**	**0**	**4**	**6**	**0**	**44818.8**	**44817.4**	**1.4**	**0.07**	*
132	**P11-10(1-2-0-0-6-5-0)**	**1**	**2**	**0**	**0**	**6**	**5**	**0**	**44936.4**	**44938.5**	**-2.1**	**0.10**	
133	P12-1(1-2-0-1-5-2-0)	1	2	0	1	5	2	0	44182.8	44182.8	0.0	0.60	*
134	P12-2(1-2-0-1-6-2-0)	1	2	0	1	6	2	0	44344.8	44344.9	-0.1	1.46	*
135	P12-3(1-2-0-1-7-2-0)	1	2	0	1	7	2	0	44506.8	44507.0	-0.2	0.48	*
136	P12-4(1-2-0-1-5-4-0)	1	2	0	1	5	4	0	44588.4	44589.2	-0.8	0.77	*
137	P12-5(1-2-0-1-5-5-0)	1	2	0	1	5	5	0	44792.4	44792.3	0.1	0.23	*
138	P12-6(1-2-0-1-6-5-0)	1	2	0	1	6	5	0	44953.2	44954.5	-1.3	0.08	*

The red highlighted species (21 species with different mass, but it includes 12 pairs of isobaric species) are the MS alone. The bolded are the isobaric species (32 pairs).

A, P, S, O in the Modifications column represents acetylation, phosphorylation, succinimide formation, oxidation, respectively. Hex, GlcNAc, NeuAc refers hexose, N-acetylhexosamine, N-acetylneuraminic acid / sialic acid, respectively.

* means the species undetected by Bones et al.

Table S3. Analysis of ovomucoid species.

No.	ID	Glycan composition			Exp. Mass Da	Theor. Mass Da	Δm Da	Ratio %
		Hex	GlcNAc	NeuAc				
1	P1-1(23-14-0)	23	14	0	26654.6	26654.2	-0.4	0.63
2	P1-2(22-15-0)	22	15	0	26696.1	26695.2	-0.9	0.62
3	P1-3(21-16-0)	21	16	0	26737.7	26736.3	-1.4	0.58
4	P1-4(20-17-0)	20	17	0	26777.0	26777.3	0.3	0.51
5	P1-5(19-18-0)	19	18	0	26816.4	26818.4	2.0	0.72
6	P1-6(18-19-0)	18	19	0	26858.4	26859.4	1.0	0.98
7	P1-7(17-20-0)	17	20	0	26901.8	26900.5	-1.3	0.85
8	P1-8(19-19-0)	19	19	0	27019.0	27021.6	2.6	1.06
9	P1-9(18-20-0)	18	20	0	27061.7	27062.6	0.9	1.62
10	P1-10(17-21-0)	17	21	0	27101.9	27103.7	1.8	1.20
11	P1-11(20-19-0)	20	19	0	27182.4	27183.7	1.3	0.90
12	P1-12(19-20-0)	19	20	0	27223.4	27224.8	1.4	1.47
13	P1-13(18-21-0)	18	21	0	27264.2	27265.8	1.6	2.09
14	P1-14(17-22-0)	17	22	0	27307.9	27306.9	-1.0	1.29
15	P1-15(20-20-0)	20	20	0	27385.4	27386.9	1.5	1.13
16	P1-16(19-21-0)	19	21	0	27426.6	27428.0	1.4	1.96
17	P1-17(18-22-0)	18	22	0	27468.4	27469.0	0.6	2.59
18	P1-18(17-23-0)	17	23	0	27508.7	27510.1	1.4	1.63
19	P1-19(15-25-0)	15	25	0	27591.0	27592.2	1.1	1.48
20	P1-20(19-22-0)	19	22	0	27629.4	27631.2	1.8	2.67
21	P1-21(18-23-0)	18	23	0	27670.5	27672.2	1.7	2.64
22	P1-22(17-24-0)	17	24	0	27712.5	27713.3	0.8	1.78
23	P1-23(15-26-0)	15	26	0	27793.1	27795.4	2.3	1.67
24	P1-24(19-23-0)	19	23	0	27834.3	27834.3	0.0	2.61
25	P1-25(18-24-0)	18	24	0	27874.2	27875.4	1.2	3.23
26	P1-26(17-25-0)	17	25	0	27915.6	27916.5	0.9	1.48
27	P1-27(15-27-0)	15	27	0	27997.7	27998.6	0.9	1.68
28	P1-28(19-24-0)	19	24	0	28037.7	28037.5	-0.2	2.76
29	P1-29(18-25-0)	18	25	0	28078.2	28078.6	0.4	2.16
30	P1-30(17-26-0)	17	26	0	28118.4	28119.6	1.2	1.30
31	P1-31(15-28-0)	15	28	0	28200.4	28201.7	1.3	1.76
32	P1-32(19-25-0)	19	25	0	28238.7	28240.7	2.1	1.86
33	P1-33(18-26-0)	18	26	0	28279.8	28281.8	2.0	1.84
34	P1-34(17-27-0)	17	27	0	28322.4	28322.8	0.4	0.93
35	P1-35(16-28-0)	16	28	0	28361.9	28363.9	2.0	0.87

Table S3. Continued

No.	ID	Glycan composition			Exp. Mass Da	Theor. Mass Da	Δm Da	Ratio %
		Hex	GlcNAc	NeuAc				
36	P1-36(15-29-0)	15	29	0	28407.9	28404.9	-3.0	1.06
37	P1-37(19-26-0)	19	26	0	28444.0	28443.9	0.1	1.55
38	P1-38(18-27-0)	18	27	0	28485.6	28485.0	-0.6	0.93
39	P1-39(17-28-0)	17	28	0	28527.9	28526.0	-1.9	0.75
40	P1-40(16-29-0)	16	29	0	28568.0	28567.1	0.9	0.71
41	P1-41(15-30-0)	15	30	0	28605.9	28608.1	-2.3	1.03
42	P1-42(19-27-0)	19	27	0	28646.8	28647.1	-0.3	0.77
43	P1-43(18-28-0)	18	28	0	28686.1	28688.2	-2.1	0.90
44	P1-44(17-29-0)	17	29	0	28731.0	28729.2	1.8	0.50
45	P1-45(16-30-0)	16	30	0	28769.0	28770.3	-1.3	0.53
46	P1-46(15-31-0)	15	31	0	28809.4	28811.3	-1.9	0.52
47	P1-47(19-28-0)	19	28	0	28848.8	28850.3	-1.5	0.58
48	P2-1(15-13-0)	15	13	0	25154.8	25153.9	0.9	0.94
49	P2-2(14-14-0)	14	14	0	25192.9	25194.9	-2.0	0.96
50	P2-3(16-13-0)	16	13	0	25318.7	25316.0	2.7	0.79
51	P2-4(15-14-0)	15	14	0	25355.1	25357.1	-2.0	1.35
52	P2-5(14-15-0)	14	15	0	25395.9	25398.1	-2.2	1.26
53	P2-6(16-14-0)	16	14	0	25518.1	25519.2	-1.1	1.17
54	P2-7(15-15-0)	15	15	0	25558.7	25560.2	-1.5	1.33
55	P2-8(14-16-0)	14	16	0	25598.9	25601.3	-2.4	1.50
56	P2-9(13-17-0)	13	17	0	25642.8	25642.4	0.4	1.78
57	P2-10(12-18-0)	12	18	0	25682.3	25683.4	-1.1	1.45
58	P2-11(15-16-0)	15	16	0	25765.7	25763.4	2.3	1.27
59	P2-12(13-18-0)	13	18	0	25842.9	25845.5	-2.6	1.37
60	P2-13(12-19-0)	12	19	0	25883.4	25886.6	-3.2	1.31
61	P2-14(15-17-0)	15	17	0	25966.1	25966.6	-0.5	1.22
62	P2-15(14-18-0)	14	18	0	26007.8	26007.7	0.1	1.74
63	P2-16(13-19-0)	13	19	0	26045.7	26048.7	-3.0	1.71
64	P2-17(12-20-0)	12	20	0	26087.2	26089.8	-2.6	1.66
65	P2-18(12-21-0)	12	21	0	26290.1	26293.0	-2.9	1.06
66	P2-19(10-23-0)	10	23	0	26373.3	26375.1	-1.8	0.75
67	P2-20(13-21-0)	13	21	0	26453.2	26455.1	-1.9	0.84
68	P2-21(12-22-0)	12	22	0	26494.7	26496.2	-1.5	0.98
69	P2-22(13-22-0)	13	22	0	26656.9	26658.3	-1.4	0.70
70	P2-23(12-23-0)	12	23	0	26697.2	26699.4	-2.2	0.69

Table S3. Continued

No.	ID	Glycan composition			Exp. Mass Da	Theor. Mass Da	Δm Da	Ratio %
		Hex	GlcNAc	NeuAc				
71	P3-1(11-17-1)	11	17	1	25608.2	25609.3	-1.1	0.47
72	P3-2(10-18-1)	10	18	1	25649.2	25650.4	-1.2	0.56
73	P3-3(11-18-1)	11	18	1	25811.3	25812.5	-1.2	0.46
74	P3-4(10-19-1)	10	19	1	25850.9	25853.6	-2.7	0.52
75	P3-5(9-20-1)	9	20	1	25893.5	25894.6	-1.1	0.55
76	P3-6(7-22-1)	7	22	1	25974.5	25976.7	-2.2	0.49
77	P3-7(6-23-1)	6	23	1	26016.8	26017.8	-1.0	0.59
78	P3-8(5-24-1)	5	24	1	26056.4	26058.8	-2.4	0.78
79	P3-9(8-23-1)	8	23	1	26340.0	26342.1	-2.1	0.63
80	P3-10(7-24-1)	7	24	1	26380.4	26383.1	-2.7	0.58
81	P3-11(8-24-1)	8	24	1	26544.3	26545.3	-0.9	0.62
82	P3-12(9-24-1)	9	24	1	26705.7	26707.4	-1.7	0.49
83	P3-13(8-25-1)	8	25	1	26747.4	26748.4	-1.0	0.60
84	P3-14(9-25-1)	9	25	1	26908.9	26910.6	-1.7	0.47

The red highlighted species (15 species) are the MS alone.

Hex, GlcNAc, NeuAc refers hexose, N-acetylhexosamine, N-acetylneuraminic acid / sialic acid, respectively.

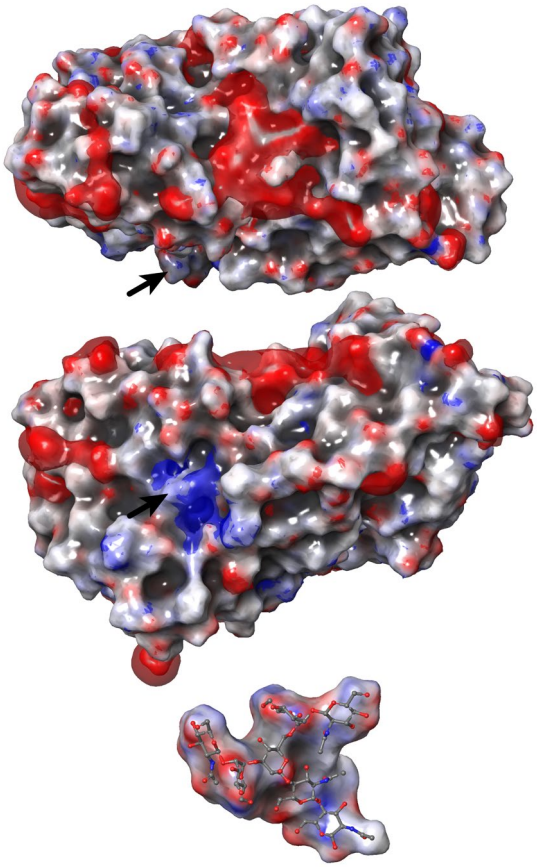

Figure S1. Two complementary views of OVA crystal structure (PDB id: 1OVA) showing isopotential surfaces at -4kT/e (with semi-transparent red surfaces) and location of the glycosylation site (with a black arrow). A biantennary Hex3GlcNAc4 structure is shown at the bottom as a reference.

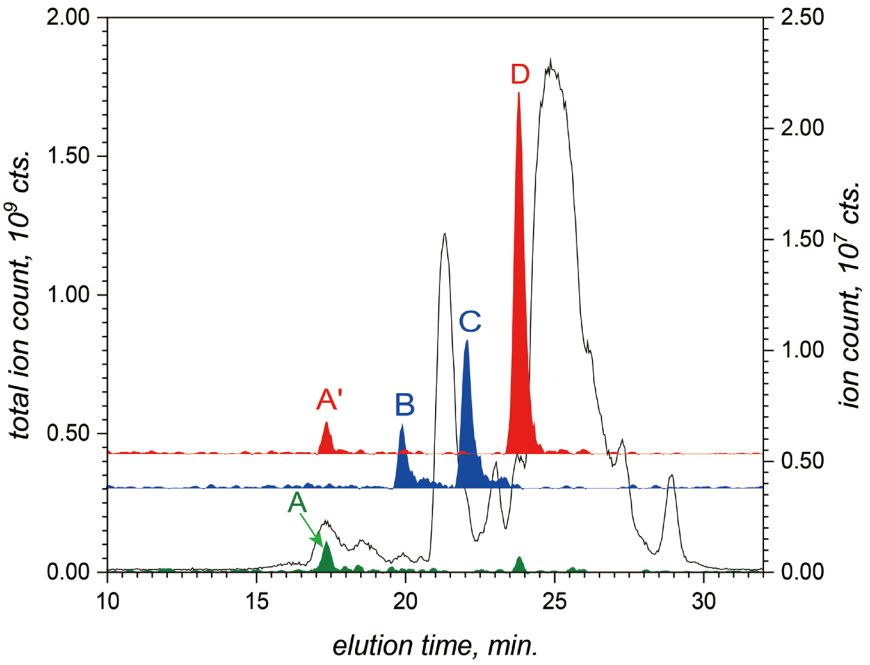

Figure S2. Influence of phosphorylation on OVA elution in anion-exchange chromatography. The extracted ion chromatograms for OVA glycoform $Hex_8GlcNAc_8NeuAc_0$ exhibiting different levels of phosphorylation (green: non-phosphorylated; blue: mono-phosphorylated; and red: bis-phosphorylated).