Supporting Information:

Fe_3O_4@PANI: A Magnetic Polyaniline Nanomaterials for Highly Specific and Handy Enrichment of Intact N-glycopeptides

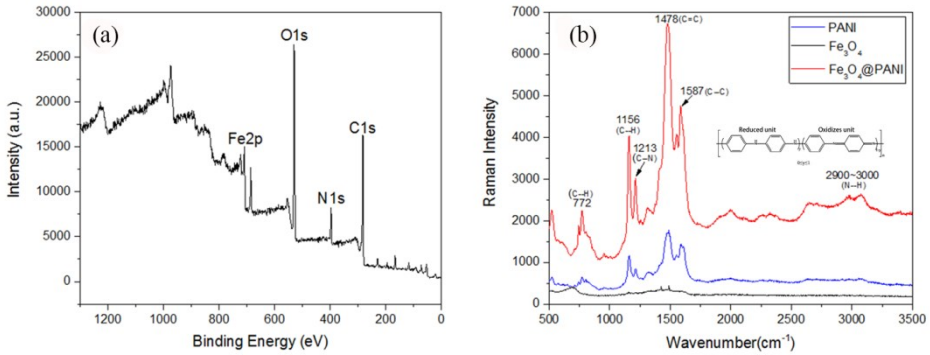

Fig.S1. The XPS spectrum (a) and Raman spectrum (b), structure (inset in b) of Fe_3O_4@PANI.

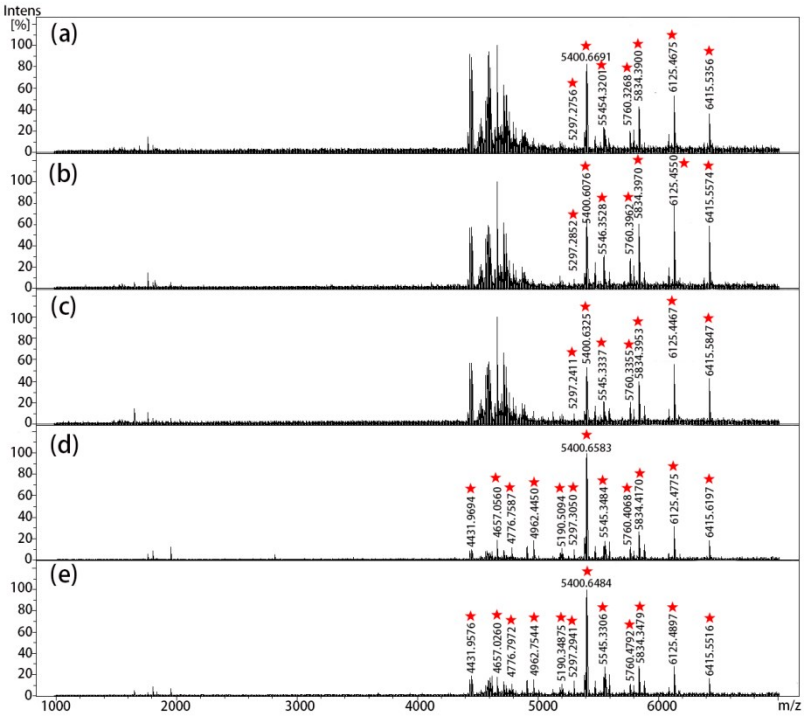

Fig.S2. Mass spectra of the Fe_3O_4@PANI-enriched N-glycopeptides from the tryptic digests of bovine fetuin (8 pmol) with different content of acetonitrile in enrichment solutions and 0.025% $NH_3 \cdot H_2O$ as eluent. The enrichment solutions were 20%(a), 40%(b), 60%(c), 80%(d), and 90% (e) , respectively. Red star diamond: N-glycopeptides.

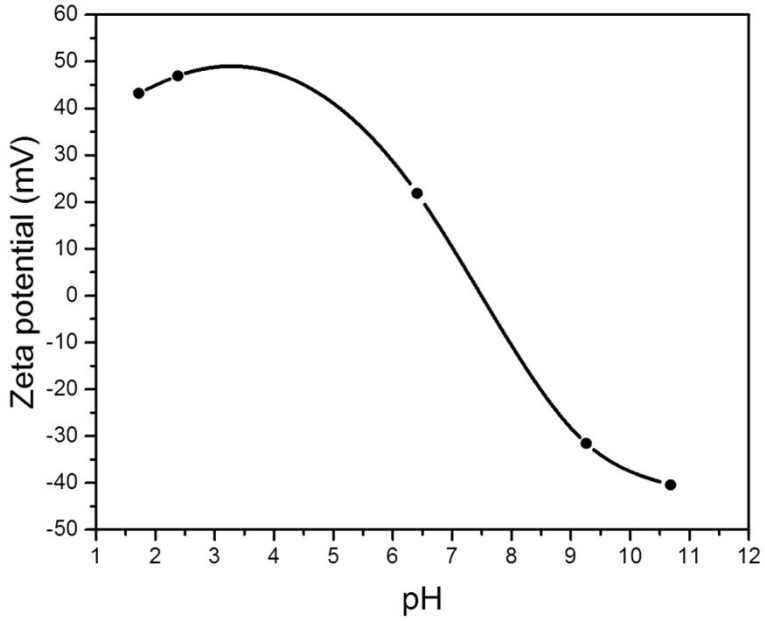

Fig.S3. The zeta potentials of Fe_3O_4@PANI dispersed in enrichment solution with different pH .

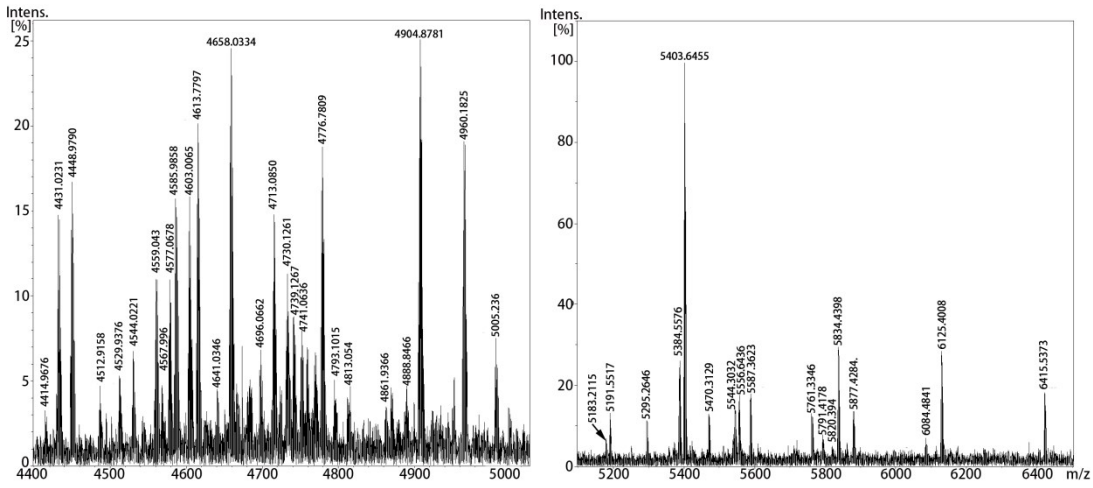

Fig.S4. The zoomed mass spectra of Fe_3O_4@PANI-enriched peptides and glycopeptides derived from the tryptic digests of fetuin.

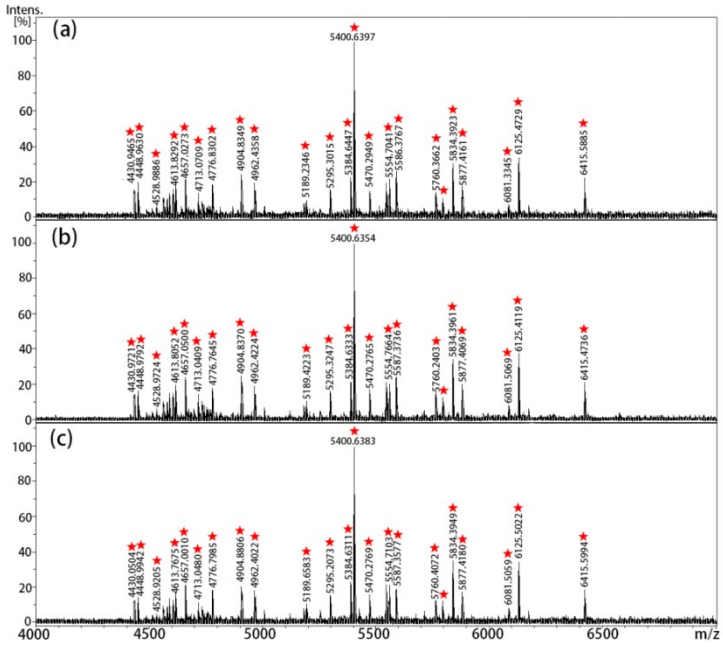

Fig.S5. The intra-day reproducibility of Fe_3O_4@PANI enrichment approach from the tryptic digests of bovine fetuin (8 pmol). 38 (a), 40 (b), and 36 (c) of N-glycopeptides were detected in three repeated experiments, respectively. Red star diamond: N-glycopeptides.

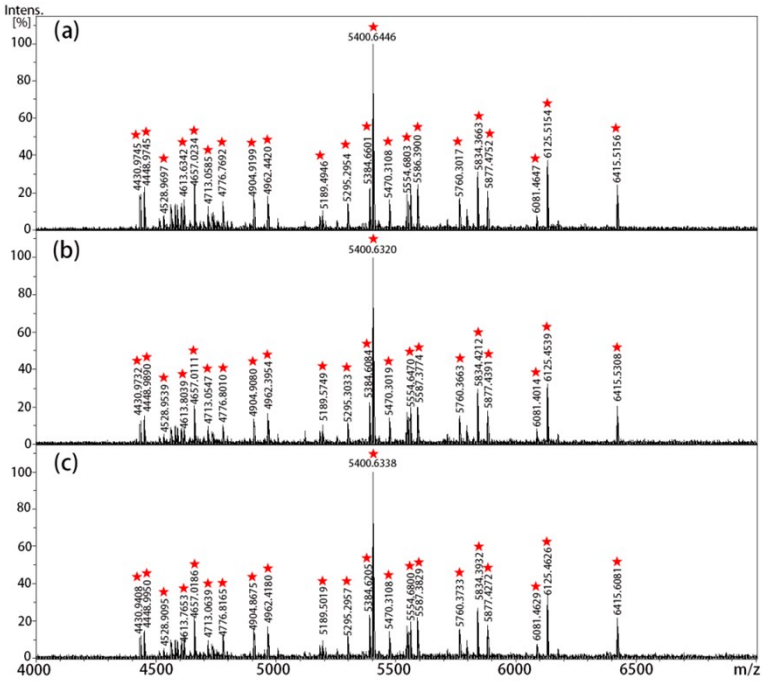

Fig.S6. The inter-day reproducibility of the Fe_3O_4@PANI enrichment approach from the tryptic digests of bovine fetuin (8 pmol). 40 (a), 39 (b), and 37 (c) of N-glycopeptides were detected in three repeated experiments, respectively. Red star diamond: N-glycopeptides.

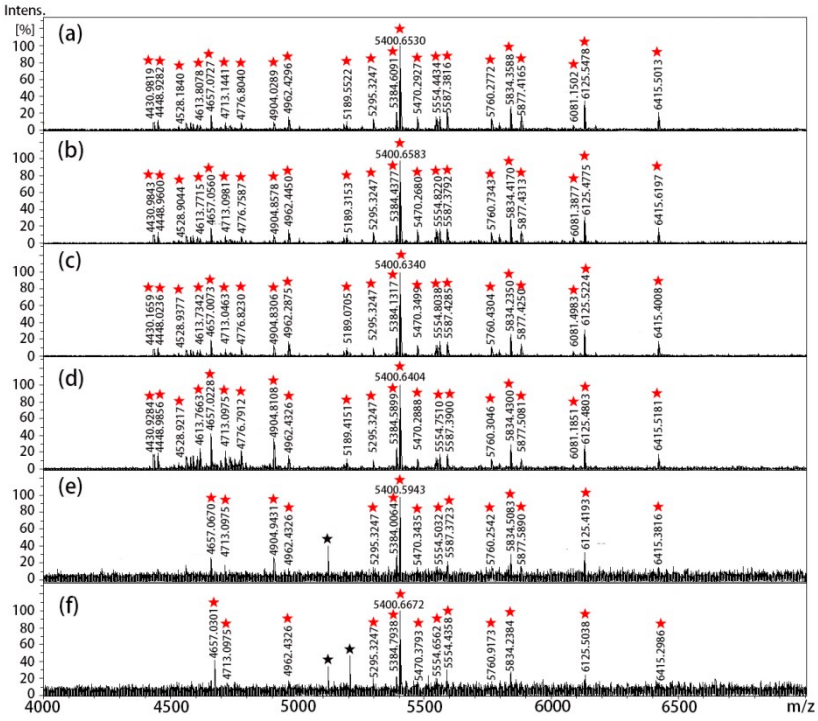

Fig.S7. Mass spectra of the Fe_3O_4@PANI-enriched N-glycopeptides from different amounts of bovine fetuin tryptic digests (i.e., 1.6 pmol (a), 0.8 pmol (b), 0.4 pmol (c), 0.2 pmol (d), 0.1pmol (e), and 50 fmol (f), respectively). Red star diamond: N-glycopeptides.; star symbol: electric noise.

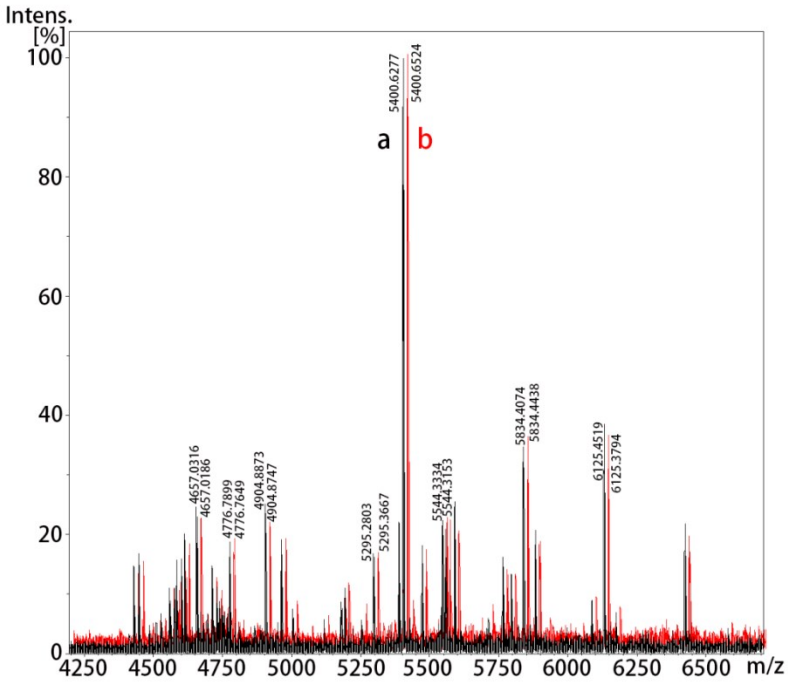

Fig.S8. The stacked mass spectra of the N-glycopeptides enriched once (a, black) and twice (b, red) by Fe_3O_4@PANI from the tryptic digests of bovine fetuin (8 pmol).

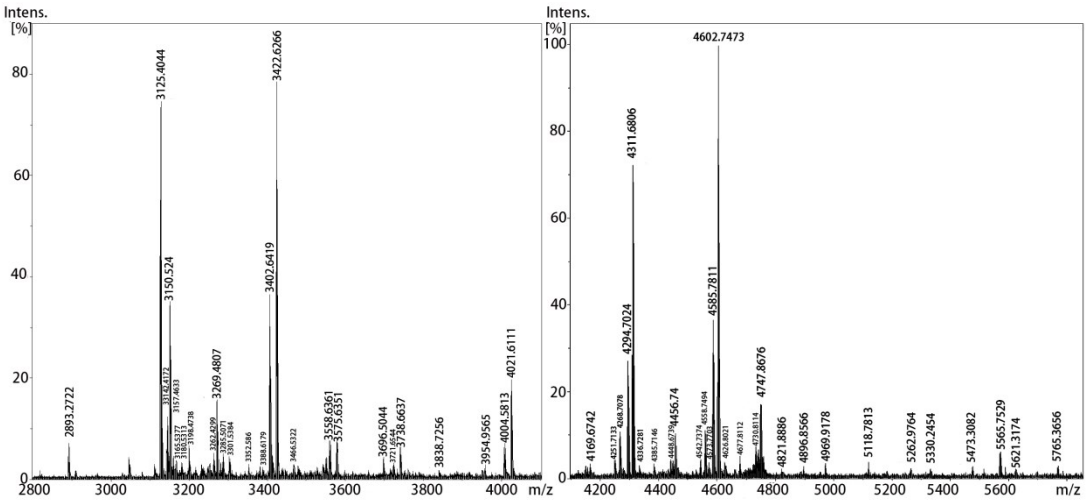

Fig.S9. The zoomed mass spectra of Fe_3O_4@PANI-enriched peptides and glycopeptides derived from the tryptic digests of transferrn.

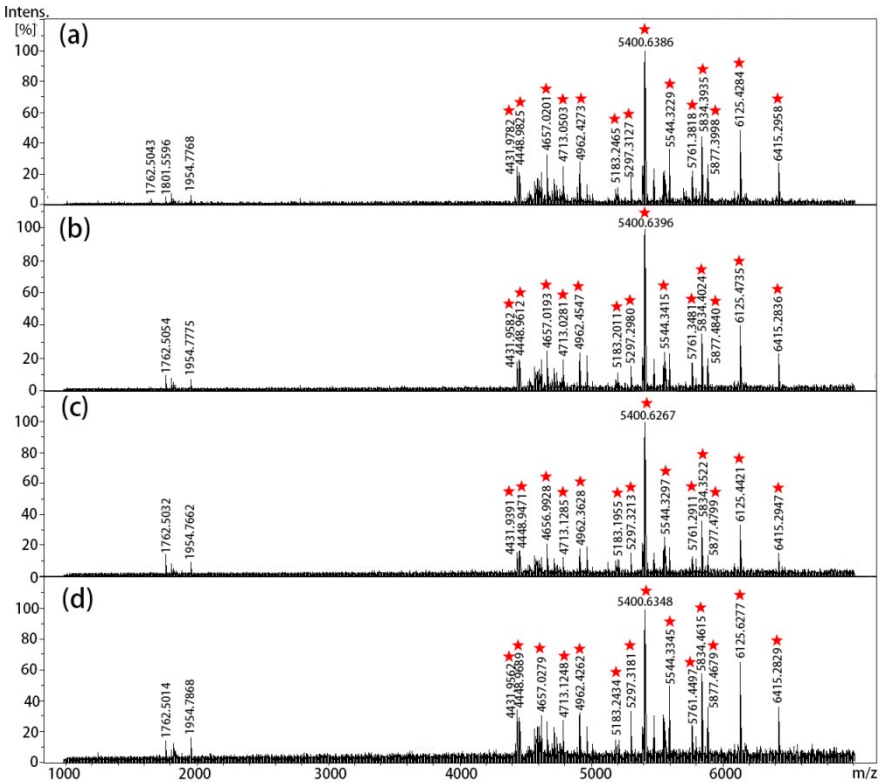

Fig.S10. Mass spectra of the Fe_3O_4@PANI-enriched N-glycopeptides from the tryptic digests of the mixtures of fetuin and albumin with the ratio of 1:1(a) , 1:20(b) , 1:50(c) and 1:70(d), respectively . Red star diamond: N-glycopeptides.

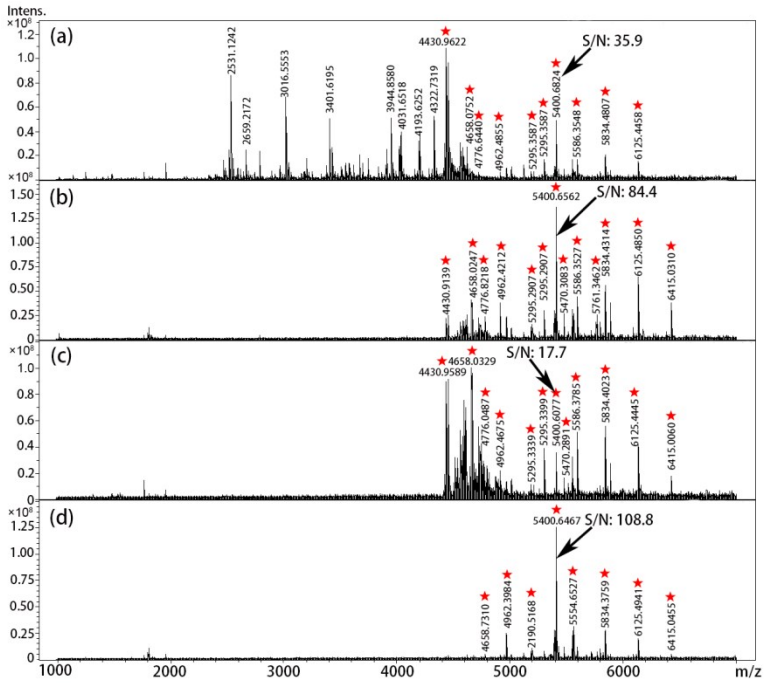

Fig.S11. Mass spectra of peptides and glycopeptides derived from the tryptic digests of bovine fetuin (8 pmol, a), Fe_3O_4@PANI(b)-, g-C_3N_4(c)- and TiO_2(d)-enriched N-glycopeptides of bovine fetuin. Red star diamond: N-glycopeptides.

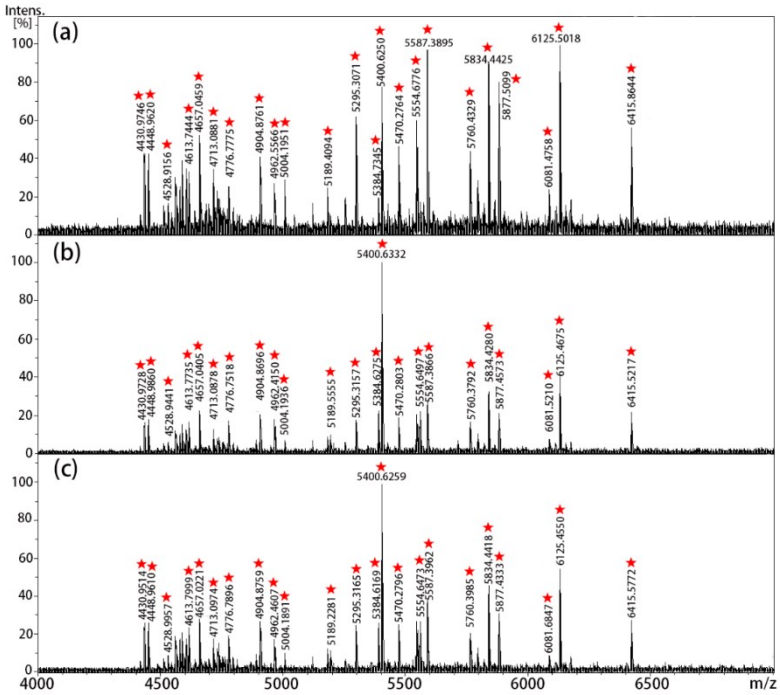

Fig.S12. Mass spectra of Fe_3O_4@PANI-enriched glycopeptides from the tryptic digests of bovine fetuin (8 pmol) under different amounts of Fe_3O_4@PANI. 0.1 mg(a), 0.2 mg (b), and 0.4 mg (c), respectively. Red star diamond: N-glycopeptides.

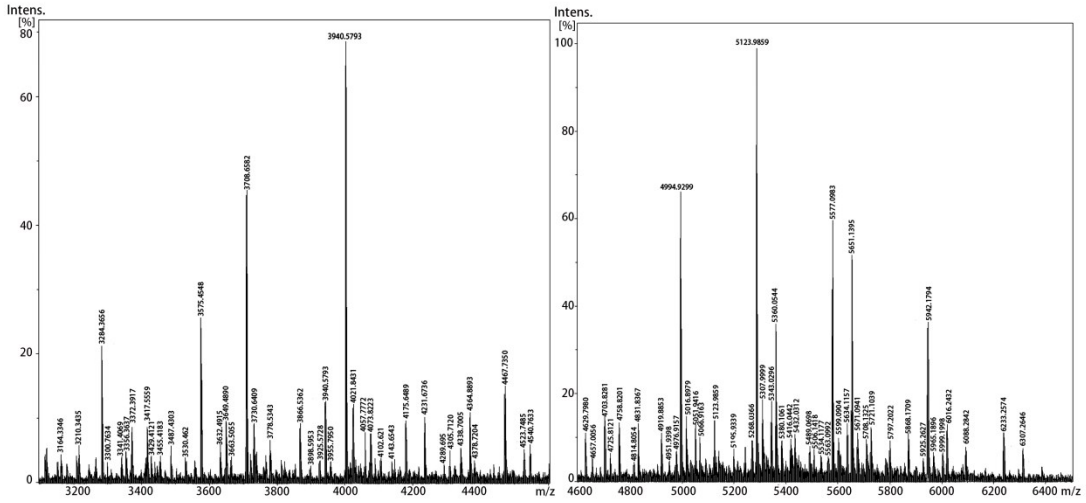

Fig.S13. The zoomed mass spectra of Fe_3O_4@PANI-enriched peptides and glycopeptides derived from the tryptic digests of haptoglobin.

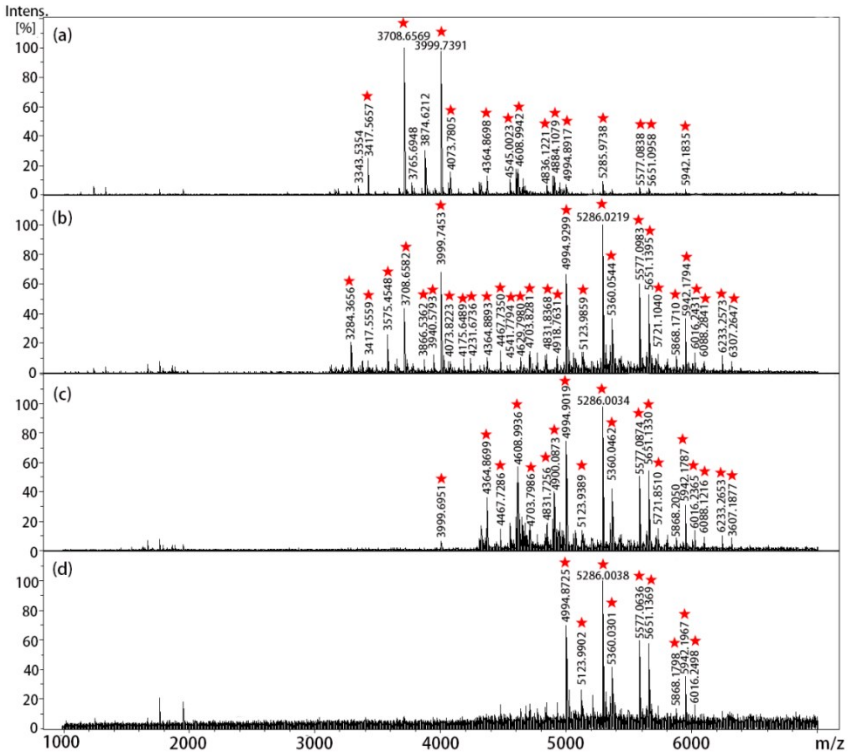

Fig.S14. Mass spectra of peptides and glycopeptides derived from the tryptic digests of haptoglobin (a), Fe_3O_4@PANI (b)-, g-C_3N_4 (c)- and TiO_2 (d)-enriched N-glycopeptides of glycopeptides. Red star diamond: N-glycopeptides.

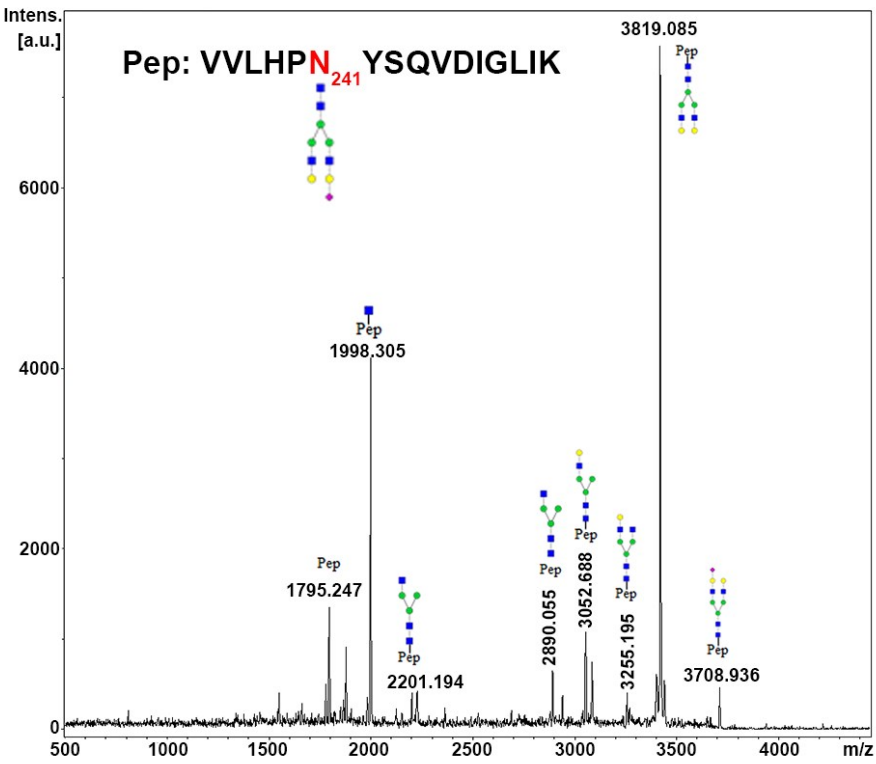

Fig.S15. Representative tandem mass spectrum of the N-glycopeptide at m/z 3708.936 of haptoglobin glycopeptide**.** Blue square, N-acetylglucosamine residue; green circle, mannose residue; yellow circle, galactose residue; red triangle, fucose residue, respectively. Red star diamond: N-glycopeptides..

Table S1. Proposed structures of the Fe_3O_4@PANI-enriched N-glycopeptides from bovine fetuin tryptic digests.

Groups	Experimental mass (Da)	Theoretical glycopeptide mass (Da)	Mass deviation (Da)	Accuracy (ppm)	Glycoform mass (Da)	Glycan structure formula
KLCPDCPLLAPLN$_{156}$DSR (MW 1867.9244 Da, 1 missed cleavage)						
1	4613.7797	4613.877	0.0973	21.09	2858.984	H1N1F1S5+M3N2
	4730.1261	4729.961	0.1651	34.91	2975.068	H1N1F3S3+M3N2
2	4641.0346	4640.924	0.1106	23.83	2886.032	H1N4F1S3+M3N2
3	4776.8909	4776.951	0.0601	12.58	3022.058	H2N1F3S4+M3N2
	5183.2115	5183.008	0.2035	39.26	3428.216	H2N3F3S4+M3N2
	4512.9158	4512.903	0.0128	2.84	2758.010	H2N4F3S1+M3N2
4	4793.1015	4792.945	0.1565	32.65	3038.052	H3N1F2S4+M3N2
5	4559.0430	4558.872	0.1710	37.51	2803.979	H3N2F1S3+M3N2
	4414.9676	4414.854	0.1136	25.73	2659.961	H3N2F4S1+M3N2
6	4585.9858	4585.919	0.0668	14.57	2831.026	H3N5F1S1+M3N2
7	5834.4398	5834.368	0.0718	12.31	4079.476	H3N9S3+M3N2
8	4813.0540	4812.873	0.1810	37.61	3056.785	H4N1F3S3+M3N2
9	4577.0678	4576.907	0.1608	35.13	2822.014	H4N2F4S1+M3N2
10	6084.4841	6084.337	0.1471	24.18	4329.545	H4N8S4+M3N2
11	4739.1267	4738.960	0.1667	35.18	2984.067	H5N2F4S1+M3N2
12	4696.0662	4695.893	0.1732	36.88	2941.000	H6N1S3+M3N2
13	4713.0850	4712.908	0.1770	37.56	2958.015	H3F2S4+M3N2
14	6417.5373	6417.026	0.5113	79.68	4660.634	H8N5F2S4+M3N2
LCPDCPLLAPLN$_{156}$DSR(MW 1625.7905 Da)						
1	4544.0221	4543.824	0.1981	43.60	2917.026	H1N2F2S4+M3N2

	4658.0334	4657.867	0.1664	35.72	3031.069	H1N4S4+M3N2
2	4888.8466	4889.014	0.1674	34.24	3262.216	H1N8F2S1+M3N2
3	4529.9376	4529.845	0.0926	20.44	2903.047	H2N4F2S2+M3N2
4	4904.8781	4905.009	0.1309	26.69	3278.211	H2N8F1S1+M3N2
5	5544.3332	5544.209	0.1242	22.40	3917.411	H7N5F4S1+M3N2
6	4603.0065	4602.861	0.1455	31.61	2976.063	H3N5S2+M3N2
7	4430.0231	4430.077	0.0539	12.17	2369.843	H3N2F1S3+M3N2
8	4448.9790	4448.812	0.167	37.54	2822.014	H4N2F4S1+M3N2
9	4960.1825	4960.002	0.1805	36.39	3333.204	H5N3F5S1+M3N2
10	4567.9960	4567.798	0.198	43.35	2941.000	H6N1S3+M3N2
11	5791.4178	5791.242	0.1758	30.36	4164.444	H6N2F3S5+M3N2
12	4741.0636	4740.903	0.1606	33.88	3114.105	H6N4F1S1+M3N2
	5470.3129	5470.172	0.1409	25.76	3843.374	H6N4F4S2+M3N2
	5761.3346	5761.157	0.1776	30.83	4134.469	H6N4F4S3+M3N2
13	6125.4008	6125.679	0.2782	45.42	4498.581	H7N5F2S4+M3N2
VVHAVEVALATFNAESN$_{176}$GSYLQLVEISR(MW 3015.5616 Da)						
1	5384.5576	5384.420	0.1376	25.56	2367.846	H3N2F2S1+M3N2
	5400.6583	5400.414	0.2443	45.24	2383.841	H4N2F1S1+M3N2
2	5555.7028	5555.509	0.1938	34.88	2538.935	H1N3F4S1+M3N2
3	5587.3623	5587.499	0.1367	24.47	2570.925	H3N3F2S1+M3N2
	5295.2646	5295.383	0.1184	22.36	2278.809	H3N3S1+M3N2
RPTGEVYDIEIDTLETTCHVLDPTPLAN$_{99}$CSVR(MW 3670.7332 Da)						
1	5820.3940	5820.539	0.1450	24.91	2262.814	H2N3F1S1+M3N2
2	5877.4084	5877.561	0.1526	25.96	2319.836	H2N4S1+M3N2

Table S2. Proposed structures of the Fe_3O_4@PANI-enriched N-glycopeptides from transferrin tryptic digests.

Groups	Experimental mass (Da)	Theoretical glycopeptide mass (Da)	Mass deviation (Da)	Accuracy (ppm)	Glycoform mass (Da)	Glycan structure formula
$IN_{491}HCR$(MW 641.3268 Da)						
1	3269.2807	3269.265	0.0157	4.80	2626.951	H1N2F4S2+M3N2
2	3180.5313	3180.429	0.1023	32.17	2537.915	H1N3F2S2+M3N2
3	3150.5240	3150.555	0.0310	9.84	2507.941	H1N5F3+M3N2
4	3352.5860	3352.514	0.0720	21.48	2710.000	H1N6F1S1+M3N2
5	3575.6351	3575.535	0.1001	28.00	2933.021	H2N2F1S4+M3N2
	3721.6544	3721.593	0.0614	16.50	3079.079	H2N2F2S4+M3N2
	3285.5071	3285.360	0.1471	44.77	2642.946	H2N2F3S2+M3N2
6	3165.5377	3165.429	0.1087	34.34	2522.915	H2N5S1+M3N2
7	3301.5384	3301.455	0.0834	25.26	2658.941	H3N2F2S2+M3N2
	3738.6637	3738.608	0.0557	14.90	3096.094	H3N2F3S3+M3N2
8	3125.4044	3125.323	0.0814	26.05	2482.909	H3N4F2+M3N2
9	3696.5044	3696.361	0.1434	38.79	3054.047	H4N1F1S4+M3N2
10	4336.7281	4336.594	0.1341	30.92	3694.280	H4N2F2S5+M3N2
11	3198.4738	3198.339	0.1348	42.15	2555.925	H4N5+M3N2
12	3838.7256	3838.572	0.1536	40.01	3196.158	H4N6F1S1+M3N2
13	3422.6266	3422.581	0.0456	13.32	2780.988	H5N1F4S1+M3N2
	4004.5813	4004.472	0.1093	27.29	3362.158	H5N1F2S4+M3N2
14	4312.6806	4312.562	0.1186	27.50	3669.248	H6N1F1S5+M3N2
	4602.7473	4602.805	0.0577	12.54	3960.491	H6N1F1S6+M3N2
	4021.6111	4021.487	0.1241	30.86	3379.173	H6N1F3S3+M3N2
15	4573.7903	4573.704	0.0863	18.87	3931.390	H6N3F4S3+M3N2

16	4251.7133	4251.614	0.0993	23.36	3609.300	H6N5F3S1+M3N2
17	5473.3082	5473.017	0.2912	53.21	4830.703	H6N6F2S5+M3N2
18	4385.7146	4385.599	0.1156	26.36	3743.285	H7N2F1S4+M3N2
	4677.8112	4677.715	0.0962	20.57	4035.401	H7N2F3S4+M3N2
19	4969.9578	4969.831	0.1268	25.51	4327.517	H7N2F5S4+M3N2
LCMGSGLN$_{523}$LCEPNNK (MW 1706.9063 Da)						
1	3142.4172	3142.382	0.0352	11.20	1549.565	H1N1F2+M3N2
2	3402.6419	3402.589	0.0529	15.55	1809.666	H1N3F1+M3N2
3	4448.6739	4448.781	0.1071	24.07	2856.058	H1N6F2S1+M3N2
4	4542.7374	4542.859	0.1216	26.77	2950.036	H3N2F2S3+M3N2
5	4626.8021	4626.858	0.0559	12.08	3034.105	H3N6F1S1+M3N2
6	4558.7294	4558.794	0.0646	14.17	2966.031	H4N2F1S3+M3N2
	4268.7078	4268.679	0.0288	6.75	2675.956	H4N2F3S1+M3N2
7	4585.7811	4585.802	0.0209	4.56	2993.079	H4N5F1S1+M3N2
	4730.8114	4730.839	0.0276	5.83	3138.116	H4N5S2+M3N2
	4294.7024	4294.706	0.0036	0.84	2701.983	H4N5F1+M3N2
8	4456.7400	4456.747	0.0070	1.57	2864.036	H5N5F1+M3N2
	4747.8676	4747.855	0.0126	2.65	3155.132	H5N5F1S1+M3N2
9	4821.8986	4821.861	0.0376	7.80	3229.168	H6N6F1+M3N2
10	5565.7529	5566.135	0.3821	68.65	3973.412	H7N6F1S2+M3N2
QQQHLFGSN$_{630}$VTDCSGN$_{637}$FCLFR (MW 2514.1124 Da)						
1	4896.8566	4896.949	0.0924	18.87	2495.868	H2N2S3+M3N2
2	5765.3656	5765.560	0.1944	33.72	2919.042	H3N4F1S2+M3N2
3	5262.9764	5263.101	0.1246	23.67	2400.074	H3N3F2S2+M3N2
4	5118.8913	5119.059	0.1677	32.76	2717.978	H5N5+M3N2

Table S3. Proposed structures of the Fe_3O_4@PANI-enriched N-glycopeptides from haptoglobin tryptic digests.

Groups	Experimental mass (Da)	Theoretical glycopeptide mass (Da)	Mass deviation (Da)	Accuracy (ppm)	Glycoform mass (Da)	Glycan structure formula
NLFLN$_{207}$HSEN$_{211}$ATAK（MW 1458.5898Da)						
1	3210.3435	3210.358	0.015	4.52	1751.624	[H1N2S1+M3N2]
2	3284.3656	3284.395	0.029	8.95	1825.661	[H2N3+M3N2]
3	3356.3637	3356.416	0.052	15.58	1897.682	[H1N2F1S1+M3N2]
4	3372.3917	3372.411	0.019	5.72	1913.677	[H2N2S1+M3N2]
5	3487.4303	3487.474	0.044	12.53	2028.740	[H2N4+M3N2]
6	3575.4548	3575.490	0.035	9.84	2116.756	[H2N3S1+M3N2]
7	3649.4890	3649.527	0.038	10.41	2190.793	[H3N4+M3N2]
8	3663.5055	3663.506	0.000	0.14	2204.772	[H2N2S2+M3N2]
9	3778.5343	3778.570	0.036	9.45	2319.836	[H2N4S1+M3N2]
10	3866.5362	3866.585	0.049	12.62	2407.852	[H2N3S2+M3N2]
11	3898.5953	3898.600	0.005	1.21	2439.867	[H2N1F3S2+M3N2]
12	3940.5793	3940.623	0.044	11.09	2481.889	[H3N4S1+M3N2]
13	3956.7747	3956.643	0.132	33.29	2497.909	[H2N2F4S1+M3N2]
14	4102.6210	4102.675	0.054	13.16	2643.941	[H1N1S1+M3N2]+[N1+M3N2]
15	4143.6543	4143.702	0.048	11.51	2684.968	[H3N5S1+M3N2]
16	4175.6489	4175.717	0.068	16.31	2716.983	[H3N3F3S1+M3N2]
17	4231.6736	4231.717	0.043	10.26	2772.984	[H3N4S2+M3N2]
18	4289.6950	4289.760	0.065	15.15	2831.026	[H3N5F1S1+M3N2]
19	4305.7120	4305.755	0.043	9.99	2847.021	[H1N2S1+M3N2]+[N1+M3N2] [H1N1S1+M3N2]+[N2+M3N2]
20	4338.7005	4338.765	0.065	14.87	2880.031	[H1N1+M3N2]+[H2N2+M3N2]

21	4378.7204	4378.796	0.076	17.27	2920.062	[H3N4F3S1+M3N2]
22	4467.7350	4467.808	0.073	16.34	3009.074	[H2N2S1+M3N2]+[N1+M3N2] [H1N1S1+M3N2]+[H1N2+M3N2]
23	4523.7485	4523.833	0.084	18.68	3065.100	[H3N4F2S2+M3N2]
24	4540.7633	4540.849	0.086	18.87	3082.115	[H4N4F3S1+M3N2]
25	4629.7980	4629.860	0.062	13.39	3171.126	[H1N1S1+M3N2]+[H2N2+M3N2] [H2N2S1+M3N2]+[H1N1+M3N2]
26	4703.8281	4703.897	0.069	14.65	3245.163	[H2N2+M3N2]+[H2N2+M3N2]
27	4725.8121	4725.892	0.080	16.91	3267.159	[H3N5S3+M3N2]
28	4758.8201	4758.902	0.082	17.21	3300.169	[H2N2S2+M3N2]+[N1+M3N2] [H1N1S2+M3N2]+[H1N2+M3N2] [H1N1S1+M3N2]+[H1N2S1+M3N2]
29	4814.8054	4814.928	0.123	25.46	3356.195	[H3N4F2S3+M3N2]
30	4831.8367	4831.944	0.107	22.21	3373.211	[H4N4F3S2+M3N2]
31	4919.8853	4919.960	0.075	15.18	3461.227	[H4N3F3S3+M3N2]
32	4976.9157	4976.981	0.065	13.12	3518.248	[H4N4F2S3+M3N2]
33	4994.9299	4994.993	0.063	12.63	3536.259	[H2N2S1+M3N2]+[H2N2+M3N2]
34	5016.8979	5016.987	0.089	17.76	3558.254	[H3N5S4+M3N2]
35	5051.9416	5052.039	0.097	19.28	3593.305	[H2N2F4S1+M3N2]+[N1+M3N2] [H2N2F3S3+M3N2]+[N1F1+M3N2] [H2N2F2S3+M3N2]+[N1F2+M3N2]
36	5066.9163	5067.013	0.097	19.08	3608.280	[H2N1F1S2+M3N2]+[H1N2+M3N2] [H1N1F1S1+M3N2]+[H2N2S1+M3N2] [H2N1S2+M3N2]+[H1N2F1+M3N2]
37	5068.9750	5069.054	0.079	15.58	3610.321	[H1N1F3+M3N2]+[H2N2F2+M3N2] [H2N2F4+M3N2]+[H1N1F1+M3N2]

38	5123.9859	5124.034	0.048	9.39	3665.301	[H1N1S1+M3N2]+[H2N2S1+M3N2] [H1N1+M3N2]+[H2N2S2+M3N2]
39	5195.9339	5196.055	0.121	23.31	3737.322	[H2N2F1S3+M3N2]+[N1+M3N2] [H2N2S3+M3N2]+[N1F1+M3N2] [H2N2S3+M3N2]+[N1F2+M3N2]
40	5268.0366	5268.166	0.129	24.56	3809.343	[H4N4F2S4+M3N2]
41	5286.0219	5286.087	0.065	12.32	3827.354	[H2N2S2+M3N2]+[H2N2+M3N2]
42	5307.9999	5308.083	0.083	15.66	3849.350	[H3N5S5+M3N2]
43	5343.0296	5343.134	0.104	19.54	3884.401	[H2N2F4S2+M3N2]+[N1+M3N2] [H2N2F3S2+M3N2]+[N1F1+M3N2] [H2N2F2S2+M3N2]+[N1F2+M3N2]
44	5360.0544	5360.125	0.071	13.17	3901.391	[H3N3S1+M3N2]+[H2N2+M3N2] [H3N3+M3N2]+[H2N2S1+M3N2]
45	5416.0442	5416.150	0.106	19.53	3957.417	[H2N2F2S2+M3N2]+[H1N2+M3N2] [H2N2F1S2+M3N2]+[H1N2F1+M3N2] [H2N2F2S1+M3N2]+[H1N2S1+M3N2] [H2N2F1S1+M3N2]+[H1N2F1S1+M3N2]
46	5432.0312	5432.145	0.114	20.95	3973.412	[H1N1F1S1+M3N2]+[H2N2S1+M3N2] [H1N1F1+M3N2]+[H2N2S2+M3N2] [H1N1+M3N2]+[H2N2F1S2+M3N2]
47	5489.0698	5489.166	0.096	17.53	4030.433	[H2N3+M3N2]+[H2N2+M3N2]
48	5506.1418	5506.198	0.056	10.21	4047.449	[H3N3F1+M3N2]+[H2N2+M3N2] [H3N3+M3N2]+[H2N2F1+M3N2] [H3N3S2+M3N2]+[H2N2F1+M3N2]
49	5577.0983	5577.182	0.084	15.01	4118.449	[H2N2S2+M3N2]+[H2N2S1+M3N2]
50	5634.1157	5634.229	0.113	20.11	4175.496	[H2N2F4S3+M3N2]+[N1+M3N2]

						[H2N2F3S2+M3N2]+[N1F1+M3N2] [H2N2F2S2+M3N2]+[N1F2+M3N2]
51	5651.1395	5651.219	0.079	14.07	4192.486	[H3N3S2+M3N2]+[H2N2+M3N2] [H3N3+M3N2]+[H2N2S2+M3N2] [H3N3S1+M3N2]+[H2N2S1+M3N2]
52	5708.1325	5708.266	0.133	23.39	4249.533	[H2N2F2S2+M3N2]+[H1N2F2+M3N2] [H2N2F1S2+M3N2]+[H1N2F3+M3N2] [H2N2F2S1+M3N2]+[H1N2F2S1+M3N2] [H2N2F1S1+M3N2]+[H1N2F3S1+M3N2]
53	5721.1039	5721.225	0.121	21.17	4262.492	[H2N1F2S5+M3N2]+[N1+M3N2] [H2N1F1S5+M3N2]+[N1F1+NM3N2] [H2N1S5+M3N2]+[N1F2+M3N2]
54	5797.2022	5797.277	0.075	12.90	4338.544	[H3N3F1S2+M3N2]+[H2N2+M3N2]
55	5868.1709	5868.278	0.107	18.25	4409.545	[H2N2S2+M3N2]+[H2N2S2+M3N2]
56	5925.2107	5925.324	0.113	19.12	4466.591	[H2N2F4S4+M3N2]+[N1+M3N2] [H2N2F3S4+M3N2]+[N1F1+M3N2] [H2N2F2S4+M3N2]+[N1F2+M3N2]
57	5942.1794	5942.315	0.136	22.82	4483.582	[H3N3S3+M3N2]+[H2N2+M3N2] [H3N3S2+M3N2]+[H2N2S1+M3N2] [H3N3S1+M3N2]+[H2N2S2+M3N2]
58	5965.1896	5965.331	0.141	23.70	4506.598	[H1N2F2S5+M3N2]+[N1+M3N2] [H1N2F1S5+M3N2]+[N1F1+M3N2] [H1N2S5+M3N2]+[N1F2+M3N2]
59	5999.1998	5999.361	0.161	26.87	4540.628	[H2N2F2S2+M3N2]+[H1N2F2S1+M3N2] [H2N2F1S2+M3N2]+[H1N2F3+M3N2] [H2N2F1S2+M3N2]+[H1N2F3S1+M3N2]

60	6016.1432	6016.381	0.238	39.53	4557.618	[H4N4S2+M3N2]+[H2N2+M3N2] [H4N4S1+M3N2]+[H2N2S1+M3N2] [H4N4+M3N2]+[H2N2S2+M3N2]
61	6088.1842	6088.373	0.189	31.01	4629.640	[H3N3F1+M3N2]+[H2N2+M3N2] [H3N3+M3N2]+[H2N2F1+M3N2]
62	6233.1574	6233.410	0.253	40.52	4774.677	[H3N3S3+M3N2]+[H2N2S1+M3N2] [H3N3S2+M3N2]+[H2N2S2+M3N2]
63	6307.2246	6307.447	0.222	35.26	4848.714	[H4N4S3+M3N2]+[H2N2+M3N2] [H4N4S2+M3N2]+[H2N2S1+M3N2] [H4N4S1+M3N2]+[H2N2S2+M3N2]
VVLHPN$_{241}$YSQVDIGLIK（MW 1795.1066Da)						
1	3417.5559	3417.593	0.037	10.86	1622.582	[H2N2+M3N2]
2	3708.6582	3708.688	0.030	8.04	1913.677	[H2N2S1+M3N2]
3	3730.7409	3730.793	0.052	13.96	1694.603	[H1N1F1S1+M3N2]
4	3766.6788	3766.730	0.051	13.59	1971.719	[H2N3F1+M3N2]
5	3999.7453	3999.783	0.038	9.43	2204.772	[H2N2S2+M3N2]
6	4057.7772	4057.825	0.048	11.78	2262.814	[H2N3F1S1+M3N2]
7	4073.8223	4073.820	0.002	0.56	2278.809	[H3N3S1+M3N2]
8	4364.8293	4364.916	0.087	19.86	2569.905	[H3N3S2+M3N2]
9	4657.0056	4657.031	0.025	5.45	2862.020	[H3N3F2S2+M3N2]