Supplementary Table
Supplementary Table 1
Compositions of 24 directly measured glycan peaks by UPLC

Glycan peak	Composition	<b>Proposed Structure</b>
GP1	H3N3F1	
GP2	H3N4	
GP3	H3N5	
GP4	H3N4F1	
GP5	H5N2	
GP6	H3N5F1	
GP7	H4N4	

GP8	H4N4F1(6)	
GP9	H4N4F1(3)	
GP10	H4N5F1(6)	
GP11	H4N5F1(3)	
GP12	H5N4	
GP13	H5N5	
GP14	H5N4F1	
GP15	H5N5F1	

		• <b>••</b> ••
GP16	H4N4F1S1(3)	<b></b>
GP17	H5N4S1	
GP18	H5N4F1S1	
GP19	H5N5F1S1	
GP20	H5N4F2S1	
GP21	H5N4S2	<b>♦</b> — <b>8</b>
GP22	H5N5S2	• • • • • • • • • • • • • • • • • • •
GP23	H5N4F1S2	
GP24	H5N5F1S2	

Note: H: hexose, N: N-acetylhexosamine; F: fucose, S: sialic acid.

**Supplementary Table 2** 

Derived glycan traits based on the glycan structure

Derived traits	Description	Formula
GPN	Profortion of neutral glycans in total IgG glycans	GP1+GP2+GP3+GP4+GP5+GP6+GP7+GP8+GP9+GP10+GP11+GP12+GP13+GP14+GP15
<b>S</b> 1	Profortion of monosialylated glycans in total IgG glycans	GP16+GP17+GP18+GP19
32	Profortion of disialylated glycans in total IgG glycans	GP21+GP22+GP23+GP24
GPS	Profortion of sialylated glycans in total IgG glycans	GPS1+GPS2
G0	Proportion of agalactosylated glycans in total IgG glycans	GP1+ GP2+ GP3+ GP4+ GP6

G1	Proportion of monogalactosylated glycans in total IgG glycans	GP7+ GP8+ GP9+ GP10+ GP11
G2	Proportion of diagalactosylated glycans in total IgG glycans	GP12+ GP13+ GP14+ GP15
F	Proportion of fucosylated glycans in total IgG glycans	GP1+ GP4+ GP6+ GP8+ GP9+ GP10+ GP11+ GP14+ GP15+ GP16+ GP18+ GP19+ GP23+ GP24
FN	Proportion of fucosylated glycans in total neutral IgG glycans	(GP1+ GP4+ GP6+ GP8+ GP9+ GP10+ GP11+ GP14+ GP15)/GPN*100
FS	Proportion of fucosylated glycans in total sialylated IgG glycans	(GP16+ GP18+ GP19+ GP23+ GP24)/GPS*100
В	Proportion of bisecting glycans in total IgG glycans	GP3+ GP6+ GP10+ GP11+ GP13+ GP15+ GP19+ GP22+ GP24

BN	Proportion of bisecting glycans in neutral IgG glycans	(GP3+ GP6+ GP10+ GP11+ GP13)/GPN*100
BS	Proportion of bisecting glycans in sialylated IgG glycans	(GP19+ GP22+ GP24)/GPS*100
FG0	Proportion of fucosylated agalactosylated glycans in total IgG glycans (glycan peak 4)	GP4
FG1	Proportion of fucosylated monogalactosylated glycans in total IgG glycans	GP8+GP9
FG2	Proportion of fucosylated diagalactosylated glycans in total IgG glycans (glycan peak 14)	GP14

Gal-ratio The relative intensity of FG0/(FG1+FG2\*2)
IgG fucosylated
galactosylation

Supplementary Table 3

The sensitivity and specificity of potential glyco-biomarkers in training cohort, validation cohort and combined cohort

	Training cohort			
	AUC	95% CI	Sensitivity	Specificity
GPN	0.72	0.65 to 0.78	86.36%	50.93%
GPS	0.71	0.65 to 0.78	86.36%	50.93%
S2	0.76	0.69 to 0.82	72.73%	70.81%
Glyco- model	0.80	0.74 to 0.86	75.00%	73.29%

	Validation cohort			
	AUC	95% CI	Sensitivity	Specificity
GPN	0.69	0.59 to 0.79	61.54%	68.24%
GPS	0.69	0.59 to 0.79	48.72%	81.18%
S2	0.72	0.62 to 0.82	51.28%	89.41%

Glycomodel 0.77 0.68 to 0.86 66.67% 76.47%

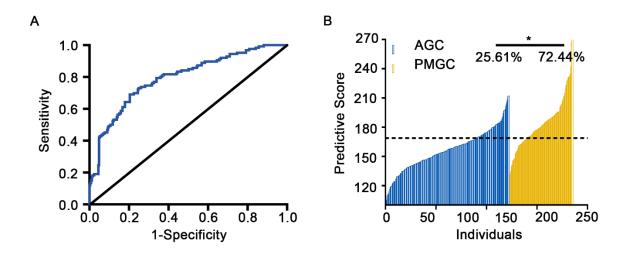
	Combined cohort			
	AUC	95% CI	Sensitivity	Specificity
GPN	0.71	0.65 to 0.76	66.93%	66.26%
GPS	0.71	0.65 to 0.76	67.72%	66.26%
S2	0.74	0.69 to 0.80	68.50%	69.92%
Glyco- model	0.79	0.74 to 0.84	72.44%	74.39%

Supplementary Table 4

The sensitivity and specificity of serum tumor biomarkers in combined cohort

	Combine cohort			
	AUC	95% CI	Sensitivity	Specificity
CEA	0.54	0.47 to 0.61	34.78%	73.33%
CA19-9	0.63	0.56 to 0.70	45.05%	80.79%
CA125	0.63	0.55 to 0.71	38.46%	86.84%
CA72-4	0.62	0.54 to 0.70	47.22%	76.22%

## **Supplementary Figure**



**Figure S1: Efficacy prediction of discriminate glyco-model of combined cohort.** Plots of ROC result (AUC= 0.79, 95%CI: 0.74 to 0.84) (A). The logistic regression predictive score for each patient of the combined cohort (B).