

Glycosylation profile of Immunoglobulin G in moderate kidney dysfunction

Supplementary Material

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Supplementary Table 1. Glycan trait and their association with eGFR. Description of 24 quantitative IgG glycosylation traits and 52 derived trait and association between all tested glycans and derived traits with CKD status and eGFR.

GROUP	Glycan	DESCRIPTION*	FORMULA*	eGFR	
				Beta [95%CI]	P
Total IgG glycans (neutral + charged)	GP1	<i>The percentage of FA1 glycan in total IgG glycans</i>	$GP1 / GP^* 100$	-0.26 [-0.74:0.22]	2.89×10^{-1}
	GP2	<i>The percentage of A2 glycan in total IgG glycans</i>	$GP2 / GP^* 100$	-0.90 [-1.42:-0.38]	6.28×10^{-4}
	GP4	<i>The percentage of FA2 glycan in total IgG glycans</i>	$GP4 / GP^* 100$	-0.60 [-1.14:-0.06]	2.87×10^{-2}
	GP5	<i>The percentage of M5 glycan in total IgG glycans</i>	$GP5 / GP^* 100$	-0.24 [-0.73:0.25]	3.30×10^{-1}
	GP6	<i>The percentage of FA2B glycan in total IgG glycans</i>	$GP6 / GP^* 100$	-1.14 [-1.71:-0.57]	8.90×10^{-5}
	GP7	<i>The percentage of A2G1 glycan in total IgG glycans</i>	$GP7 / GP^* 100$	-0.53 [-1.00:-0.06]	2.78×10^{-2}
	GP8	<i>The percentage of FA2[6]G1 glycan in total IgG glycans</i>	$GP8 / GP^* 100$	0.46 [-0.02:0.93]	5.89×10^{-2}
	GP9	<i>The percentage of FA2[3]G1 glycan in total IgG glycans</i>	$GP9 / GP^* 100$	0.07 [-0.39:0.53]	7.69×10^{-1}
	GP10	<i>The percentage of FA2[6]BG1 glycan in total IgG glycans</i>	$GP10 / GP^* 100$	-0.13 [-0.60:0.34]	5.86×10^{-1}
	GP11	<i>The percentage of FA2[3]BG1 glycan in total IgG glycans</i>	$GP11 / GP^* 100$	-0.38 [-0.88:0.11]	1.30×10^{-1}
	GP12	<i>The percentage of A2G2 glycan in total IgG glycans</i>	$GP12 / GP^* 100$	0.18 [-0.30:0.66]	4.58×10^{-1}
	GP13	<i>The percentage of A2BG2 glycan in total IgG glycans</i>	$GP13 / GP^* 100$	0.33 [-0.16:0.82]	1.91×10^{-1}
	GP14	<i>The percentage of FA2G2 glycan in total IgG glycans</i>	$GP14 / GP^* 100$	1.46 [0.85:2.07]	2.92×10^{-6}
	GP15	<i>The percentage of FA2BG2 glycan in total IgG glycans</i>	$GP15 / GP^* 100$	0.70 [0.17:1.23]	9.47×10^{-3}
	GP16	<i>The percentage of FA2G1S1 glycan in total IgG glycans</i>	$GP16 / GP^* 100$	0.51 [0.03:0.99]	3.66×10^{-2}
	GP17	<i>The percentage of A2G2S1 glycan in total IgG glycans</i>	$GP17 / GP^* 100$	-0.09 [-0.55:0.37]	7.10×10^{-1}
	GP18	<i>The percentage of FA2G2S1 glycan in total IgG glycans</i>	$GP18 / GP^* 100$	1.48 [0.89:2.07]	8.60×10^{-7}
	GP19	<i>The percentage of FA2BG2S1 glycan in total IgG glycans</i>	$GP19 / GP^* 100$	-0.11 [-0.57:0.35]	6.37×10^{-1}
	GP20+GP21		$(GP20+GP21)/GP^* 100$	0.14 [-0.14:0.42]	3.38×10^{-1}
	GP22	<i>The percentage of A2BG2S2 glycan in total IgG glycans</i>	$GP22 / GP^* 100$	0.13 [-0.32:0.58]	5.67×10^{-1}
	GP23	<i>The percentage of FA2G2S2 glycan in total IgG glycans</i>	$GP23 / GP^* 100$	0.69 [0.19:1.18]	6.63×10^{-3}
	GP24	<i>The percentage of FA2BG2S2 glycan in total IgG glycans</i>	$GP24 / GP^* 100$	0.08 [-0.38:0.53]	7.36×10^{-1}

Total IgG glycans - derived parameters	FGS/(FG+FGS)	<i>The percentage of sialylation of fucosylated galactosylated structures without bisecting GlcNAc in total IgG glycans</i>	$\frac{SUM(GP16 + GP18 + GP23)}{SUM(GP16 + GP18 + GP23 + GP8 + GP9 + GP14)} * 100$	0.76 [0.25:1.27]	3.35×10^{-3}
	FBGS/(FBG+FBGS)	<i>The percentage of sialylation of fucosylated galactosylated structures with bisecting GlcNAc in total IgG glycans</i>	$\frac{SUM(GP19 + GP24)}{SUM(GP19 + GP24 + GP10 + GP11 + GP15)} * 100$	-0.06 [-0.52:0.41]	8.11×10^{-1}
	FGS/(F+FG+FGS)	<i>The percentage of sialylation of all fucosylated structures without bisecting GlcNAc in total IgG glycans</i>	$\frac{SUM(GP16 + GP18 + GP23)}{SUM(GP16 + GP18 + GP23 + GP4 + GP8 + GP9 + GP14)} * 100$	1.01 [0.46:1.56]	2.96×10^{-4}
	FBGS/(FB+FBG+FBGS)	<i>The percentage of sialylation of all fucosylated structures with bisecting GlcNAc in total IgG glycans</i>	$\frac{SUM(GP19 + GP24)}{SUM(GP19 + GP24 + GP6 + GP10 + GP11 + GP15)} * 100$	0.24 [-0.23:0.72]	3.16×10^{-1}
	FG1S1/(FG1+FG1S1)	<i>The percentage of monosialylation of fucosylated monogalactosylated structures in total IgG glycans</i>	$\frac{GP16}{SUM(GP16 + GP8 + GP9)} * 100$	0.20 [-0.28:0.67]	4.19×10^{-1}
	FG2S1/(FG2+FG2S1+FG2S2)	<i>The percentage of monosialylation of fucosylated digalactosylated structures in total IgG glycans</i>	$\frac{GP18}{SUM(GP18 + GP14 + GP23)} * 100$	0.27 [-0.22:0.77]	2.82×10^{-1}
	FG2S2/(FG2+FG2S1+FG2S2)	<i>The percentage of disialylation of fucosylated digalactosylated structures in total IgG glycans</i>	$\frac{GP23}{SUM(GP23 + GP14 + GP18)} * 100$	-0.27 [-0.75:0.21]	2.72×10^{-1}
	FBG2S1/(FBG2+FBG2S1+FBG2S2)	<i>The percentage of monosialylation of fucosylated digalactosylated structures with bisecting GlcNAc in total IgG glycans</i>	$\frac{GP19}{SUM(GP19 + GP15 + GP24)} * 100$	-0.63 [-1.12:-0.13]	1.25×10^{-2}
	FBG2S2/(FBG2+FBG2S1+FBG2S2)	<i>The percentage of disialylation of fucosylated digalactosylated structures with bisecting GlcNAc in total IgG glycans</i>	$\frac{GP24}{SUM(GP24 + GP15 + GP19)} * 100$	-0.11 [-0.59:0.37]	6.59×10^{-1}
	$F^{total}S1/F^{total}S2$	<i>Ratio of all fucosylated (+/- bisecting GlyNAc) monosialylated and disialylated structures in total IgG glycans</i>	$\frac{SUM(GP16 + GP18 + GP19)}{SUM(GP23 + GP24)}$	0.49 [0.00:0.98]	4.77×10^{-2}
FS1/FS2	<i>Ratio of fucosylated (without bisecting GlcNAc) monosialylated and disialylated structures in total IgG</i>	$\frac{SUM(GP16 + GP18)}{GP23}$	0.17 [-0.30:0.64]	4.71×10^{-1}	

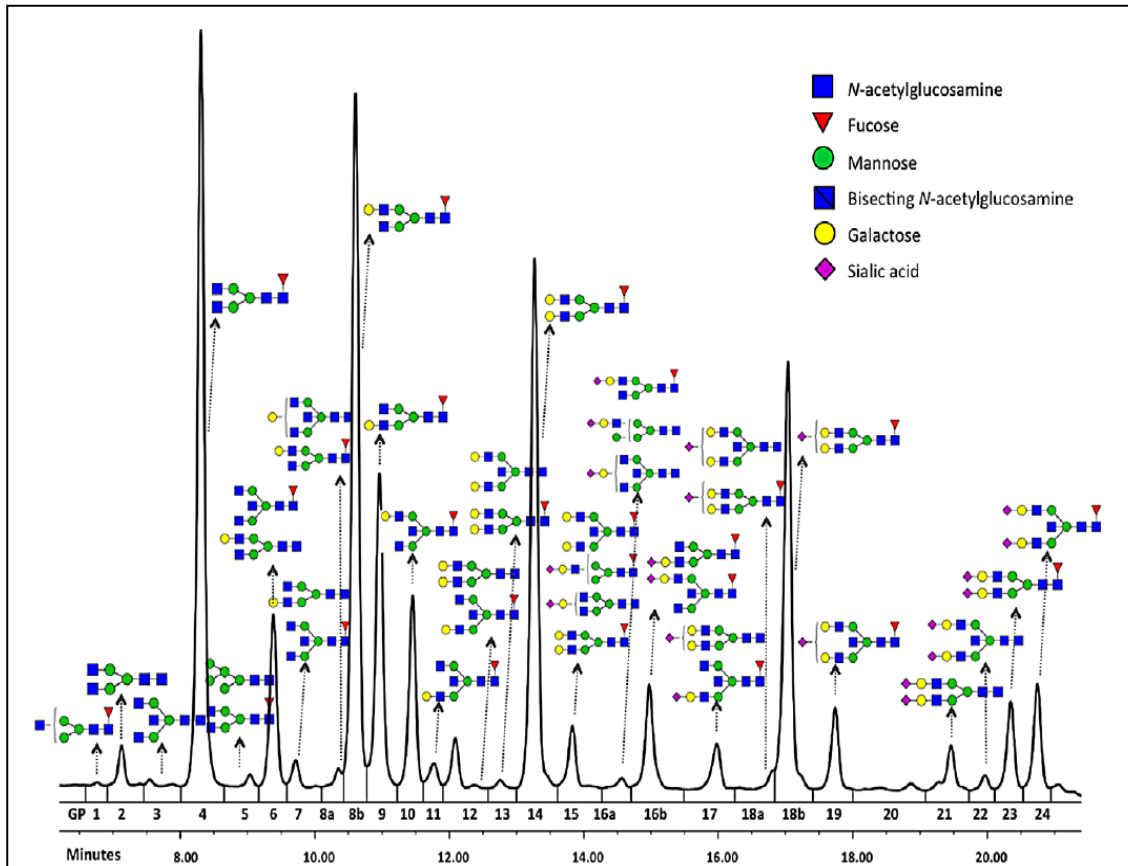
	<i>glycans</i>			
FBS1/FBS2	<i>Ratio of fucosylated (with bisecting GlcNAc) monosialylated and disialylated structures in total IgG glycans</i>	<i>GP19 / GP24</i>	-0.30 [-0.78:0.17]	2.09×10^{-1}
FBS^{total}/FS^{total}	<i>Ratio of all fucosylated sialylated structures with and without bisecting GlcNAc</i>	<i>SUM(GP19 + GP24) / SUM(GP16 + GP18 + GP23)</i>	-1.07 [-1.60:-0.54]	8.21×10^{-5}
FBS1/FS1	<i>Ratio of fucosylated monosialylated structures with and without bisecting GlcNAc</i>	<i>GP19 / SUM(GP16 + GP18)</i>	-1.12 [-1.65:-0.59]	3.48×10^{-5}
FBS1/(FS1+FBS1)	<i>The incidence of bisecting GlcNAc in all fucosylated monosialylated structures in total IgG glycans</i>	<i>GP19 / SUM(GP16 + GP18 + GP19)</i>	-1.10 [-1.63:-0.57]	4.63×10^{-5}
FBS2/FS2	<i>Ratio of fucosylated disialylated structures with and without bisecting GlcNAc</i>	<i>GP24 / GP23</i>	-0.90 [-1.42:-0.37]	8.45×10^{-4}
FBS2/(FS2+FBS2)	<i>The incidence of bisecting GlcNAc in all fucosylated disialylated structures in total IgG glycans</i>	<i>GP24 / SUM(GP23 + GP24)</i>	-0.91 [-1.44:-0.37]	8.47×10^{-4}
GP1ⁿ	<i>The percentage of FA1 glycan in total neutral IgG glycans (GPⁿ)</i>	<i>GP1 / GPⁿ * 100</i>	-0.32 [-0.81:0.16]	1.92×10^{-1}
GP2ⁿ	<i>The percentage of A2 glycan in total neutral IgG glycans (GPⁿ)</i>	<i>GP2 / GPⁿ * 100</i>	-0.91 [-1.42:-0.40]	5.02×10^{-4}
GP4ⁿ	<i>The percentage of FA2 glycan in total neutral IgG glycans (GPⁿ)</i>	<i>GP4 / GPⁿ * 100</i>	-0.90 [-1.47:-0.33]	2.04×10^{-3}
GP5ⁿ	<i>The percentage of M5 glycan in total neutral IgG glycans (GPⁿ)</i>	<i>GP5 / GPⁿ * 100</i>	-0.26 [-0.75:0.22]	2.87×10^{-1}
GP6ⁿ	<i>The percentage of FA2B glycan in total neutral IgG glycans (GPⁿ)</i>	<i>GP6 / GPⁿ * 100</i>	-1.39 [-1.98:-0.80]	3.56×10^{-6}
GP7ⁿ	<i>The percentage of A2G1 glycan in total neutral IgG glycans (GPⁿ)</i>	<i>GP7 / GPⁿ * 100</i>	-0.52 [-0.99:-0.05]	2.87×10^{-2}
GP8ⁿ	<i>The percentage of FA2[6]G1 glycan in total neutral IgG glycans (GPⁿ)</i>	<i>GP8 / GPⁿ * 100</i>	0.53 [0.02:1.04]	3.98×10^{-2}
GP9ⁿ	<i>The percentage of FA2[3]G1 glycan in total neutral IgG glycans (GPⁿ)</i>	<i>GP9 / GPⁿ * 100</i>	-0.02 [-0.48:0.45]	9.46×10^{-1}
GP10ⁿ	<i>The percentage of FA2[6]BG1 glycan in total neutral IgG glycans (GPⁿ)</i>	<i>GP10 / GPⁿ * 100</i>	-0.21 [-0.68:0.26]	3.81×10^{-1}
<i>Neutral IgG glycans</i>				

	GP11 ⁿ	The percentage of FA2[3]BG1 glycan in total neutral IgG glycans (GP ⁿ)	$GP11 / GP^n * 100$	-0.50 [-0.99:-0.01]	4.71×10^{-2}
	GP12 ⁿ	The percentage of A2G2 glycan in total neutral IgG glycans (GP ⁿ)	$GP12 / GP^n * 100$	0.13 [-0.35:0.61]	5.93×10^{-1}
	GP13 ⁿ	The percentage of A2BG2 glycan in total neutral IgG glycans (GP ⁿ)	$GP13 / GP^n * 100$	0.20 [-0.29:0.69]	4.20×10^{-1}
	GP14 ⁿ	The percentage of FA2G2 glycan in total neutral IgG glycans (GP ⁿ)	$GP14 / GP^n * 100$	1.29 [0.68:1.90]	3.06×10^{-5}
	GP15 ⁿ	The percentage of FA2BG2 glycan in total neutral IgG glycans (GP ⁿ)	$GP15 / GP^n * 100$	0.51 [-0.01:1.03]	5.55×10^{-2}
Neutral IgG glycans - derived parameters	G0 ⁿ	The percentage of agalactosylated structures in total neutral IgG glycans	$SUM(GP1^n : GP6^n)$	-1.16 [-1.76:-0.56]	1.52×10^{-4}
	G1 ⁿ	The percentage of monogalactosylated structures in total neutral IgG glycans	$SUM(GP7^n : GP11^n)$	0.36 [-0.12:0.84]	1.45×10^{-1}
	G2 ⁿ	The percentage of digalactosylated structures in total neutral IgG glycans	$SUM(GP12^n : GP15^n)$	1.20 [0.60:1.80]	8.81×10^{-5}
	F ^{n total}	The percentage of all fucosylated (+/- bisecting GlcNAc) structures in total neutral IgG glycans	$SUM(GP1^n + GP4^n + GP5^n + GP6^n + GP8^n + GP9^n + GP10^n + GP11^n + GP14^n + GP15^n)$	0.31 [-0.16:0.77]	1.93×10^{-1}
	FG0 ^{n total} /G0 ⁿ	The percentage of fucosylation of agalactosylated structures	$SUM(GP1^n + GP4^n + GP5^n + GP6^n) / G0^n * 100$	0.49 [0.01:0.98]	4.67×10^{-2}
	FG1 ^{n total} /G1 ⁿ	The percentage of fucosylation of monogalactosylated structures	$SUM(GP8^n + GP9^n + GP10^n + GP11^n) / G1^n * 100$	0.53 [0.05:1.00]	2.89×10^{-2}
	FG2 ^{n total} /G2 ⁿ	The percentage of fucosylation of digalactosylated structures	$SUM(GP14^n + GP15^n) / G2^n * 100$	0.44 [-0.04:0.92]	7.54×10^{-2}
	F ⁿ	The percentage of fucosylated (without bisecting GlcNAc) structures in total neutral IgG glycans	$SUM(GP1^n + GP4^n + GP5^n + GP8^n + GP9^n + GP14^n)$	0.58 [0.09:1.07]	2.15×10^{-2}
	FG0 ⁿ /G0 ⁿ	The percentage of fucosylation (without bisecting GlcNAc) of agalactosylated structures	$SUM(GP1^n + GP4^n + GP5^n) / G0^n * 100$	0.36 [-0.11:0.83]	1.29×10^{-1}

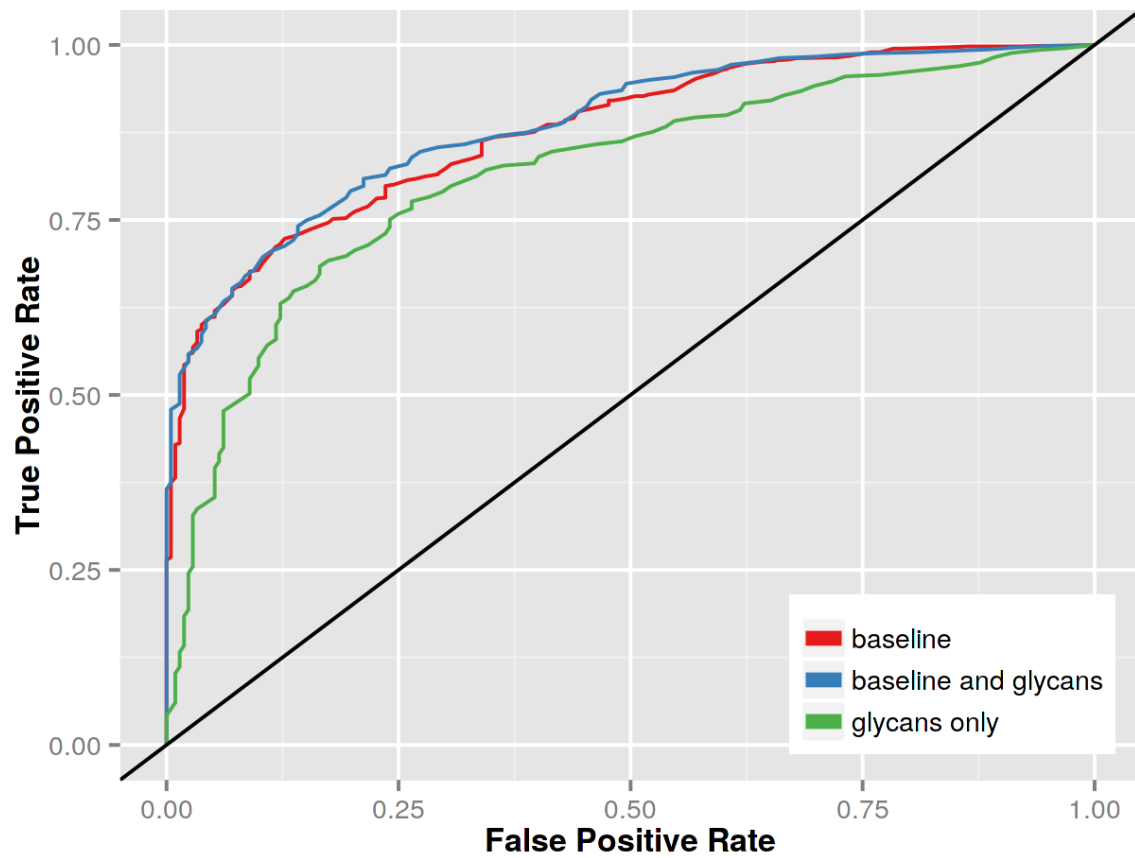
$FG1^n/G1^n$	<i>The percentage of fucosylation (without bisecting GlcNAc) of monogalactosylated structures</i>	$SUM(GP8^n + GP9^n) / G1^n * 100$	0.36 [-0.12:0.85]	1.39×10^{-1}
$FG2^n/G2^n$	<i>The percentage of fucosylation (without bisecting GlcNAc) of digalactosylated structures</i>	$GP14^n / G2^n * 100$	0.73 [0.23:1.24]	4.44×10^{-3}
FB^n	<i>The percentage of fucosylated (with bisecting GlcNAc) structures in total neutral IgG glycans</i>	$SUM(GP6^n + GP10^n + GP11^n + GP15^n)$	-0.68 [-1.19:-0.17]	8.51×10^{-3}
$FBG0^n/G0^n$	<i>The percentage of fucosylation (with bisecting GlcNAc) of agalactosylated structures</i>	$GP6^n / G0^n * 100$	-0.42 [-0.90:0.05]	7.88×10^{-2}
$FBG1^n/G1^n$	<i>The percentage of fucosylation (with bisecting GlcNAc) of monogalactosylated structures</i>	$SUM(GP10^n + GP11^n) / G1^n * 100$	-0.36 [-0.85:0.12]	1.40×10^{-1}
$FBG2^n/G2^n$	<i>The percentage of fucosylation (with bisecting GlcNAc) of digalactosylated structures</i>	$GP15^n / G2^n * 100$	-0.85 [-1.37:-0.33]	1.36×10^{-3}
FB^n/F^n	<i>Ratio of fucosylated structures with and without bisecting GlcNAc</i>	$FB^n / F^n * 100$	-0.67 [-1.17:-0.16]	9.44×10^{-3}
$FB^n/F^{n \text{ total}}$	<i>The incidence of bisecting GlcNAc in all fucosylated structures in total neutral IgG glycans</i>	$FB^n / F^{n \text{ total}} * 100$	-0.69 [-1.19:-0.18]	7.85×10^{-3}
$F^n/(B^n + FB^n)$	<i>Ratio of fucosylated non-bisecting GlcNAc structures and all structures with bisecting GlcNAc</i>	$F^n / (GP13^n + FB^n)$	0.65 [0.15:1.16]	1.09×10^{-2}
$B^n/(F^n + FB^n)$	<i>Ratio of structures with bisecting GlcNAc and all fucosylated structures (+/- bisecting GlcNAc)</i>	$GP13^n / (F^n + FB^n) * 1000$	0.18 [-0.31:0.66]	4.70×10^{-1}
$FBG2^n/FG2^n$	<i>Ratio of fucosylated digalactosylated structures with and without bisecting GlcNAc</i>	$GP15^n / GP14^n$	-0.89 [-1.41:-0.36]	9.00×10^{-4}
$FBG2^n / (FG2^n + FBG2^n)$	<i>The incidence of bisecting GlcNAc in all fucosylated digalactosylated structures in total neutral IgG glycans</i>	$GP15^n / (GP14^n + GP15^n) * 100$	-0.89 [-1.42:-0.37]	8.47×10^{-4}
$FG2^n / (BG2^n + FBG2^n)$	<i>Ratio of fucosylated digalactosylated non-bisecting GlcNAc structures and all digalactosylated structures with bisecting GlcNAc</i>	$GP14^n / (GP13^n + GP15^n)$	0.91 [0.38:1.44]	7.32×10^{-4}
$BG2^n / (FG2^n + FBG2^n)$	<i>Ratio of digalactosylated structures with bisecting GlcNAc and all fucosylated digalactosylated structures (+/- bisecting GlcNAc)</i>	$GP15^n / (GP14^n + GP15^n) * 1000$	-0.93 [-1.46:-0.39]	6.56×10^{-4}

*Previously published in Lauc et al. 2013

Supplementary figure1: UPLC analysis of the IgG glycome. An example of a UPLC chromatogram with graphical representation of glycan structures present in each chromatography peak (GP1 – GP24). *Previously published in Lauc *et al.* 2013.



Supplementary Figure 2. ROC curves illustrating the performance of regularized logistic regression model in predicting disease status for CKD cases and controls in the discovery population.



Supplementary Table 2: Comparison of Fc and Fab IgG glycopeptide by nano LC-MS/MS

MS glycans (n=96)		ULPC glycans (n=3212)	
Glycan name	Beta[95%CI]	Glycan name	Beta[95%CI]
IgG1_G2FS1	3.27 [-2.28;8.82]	GP18	1.48 [0.89;2.07]
IgG1_G2F	6.23 [-0.59;13.04]	GP14	1.46 [0.85;2.07]
IgG1_G0FNn	-1.46 [-6.98;4.07]	GP6n	-1.39 [-1.98;-0.80]
IgG1_G2Fn	5.20 [-1.39;11.79]	GP14n	1.29 [0.68;1.90]
IgG1 FBS1/FS1	-4.55 [-9.49;0.40]	FBS1/FS1	-1.12 [-1.65;-0.59]
IgG1 FBS1/(FS1+FBS1)	-5.34 [-10.45;-0.23]	FBS1/(FS1+FBS1)	-1.10 [-1.63;-0.57]
IgG1 G2n	3.44 [-3.04;9.92]	G2n	1.20 [0.60;1.80]
IgG1_G0FN	-1.15 [-6.73;4.43]	GP6	-1.14 [-1.71;-0.57]
IgG1 G0n	-0.71 [-6.81;5.38]	G0n	-1.16 [-1.76;-0.56]
IgG1 FGS1/(F+FG+FGS1)	-0.23 [-5.38;4.91]	FGS/(F+FG+FGS)	1.01 [0.46;1.56]
IgG1_G0n	-2.27 [-8.33;3.80]	GP2n	-0.91 [-1.42;-0.40]
IgG1_G0	-1.88 [-7.97;4.21]	GP2	-0.90 [-1.43;-0.38]

Supplementary Table 3: Association of total plasma glycome and eGFR

Total plasma glycan peak	Major glycan(s)	B [95% CI]	p
gly2	M5, FA2B	-1.91 [-3.42:-0.40]	0.01
gly1	FA2	-1.44 [-2.88:-0.00]	0.05
gly42	A4F1G4S4	0.89 [-0.27:2.06]	0.13
gly34	FA3G3S3	0.88 [-0.33:2.09]	0.15
gly41	A4G4S4	0.84 [-0.31:2.00]	0.15
gly6	FA2[6]BG1	-0.96 [-2.32:0.40]	0.17
gly30	A3G3S3	0.76 [-0.53:2.04]	0.25
gly16	A2BG2S1	-0.71 [-2.00:0.58]	0.28
gly40	A4G4S4	0.64 [-0.55:1.84]	0.29
gly4	FA2[6]G1	-0.74 [-2.11:0.63]	0.29
gly39	A4G4S4	0.63 [-0.61:1.87]	0.32
gly13	FA2[3]G1S1	0.60 [-0.58:1.77]	0.32
gly35	A3F1G3S3	0.67 [-0.66:2.00]	0.32
gly33	A3G3S3	0.58 [-0.62:1.78]	0.35

gly10.11	FA2G2	0.76 [-0.92:2.43]	0.38
gly36	A4G4S3	0.55 [-0.71:1.81]	0.39
gly3	A2[6]BG1	-0.53 [-1.82:0.77]	0.43
gly19	FA2BG2S1	-0.53 [-1.84:0.78]	0.43
gly9	A2BG2	-0.49 [-1.70:0.72]	0.43
gly14	FA2[3]G1S1	-0.49 [-1.78:0.81]	0.46
gly7	M6	-0.44 [-1.61:0.73]	0.46
gly38	A4F1G3S3	0.42 [-0.89:1.73]	0.53
gly37	A4G4S3	0.40 [-0.90:1.69]	0.55
gly18	FA2G2S1	0.44 [-1.07:1.94]	0.57
gly26	FA2BG2S2	-0.36 [-1.70:0.99]	0.60
gly24	A2BG2S2	0.28 [-0.99:1.55]	0.67
gly5	FA2[3]G1	-0.29 [-1.64:1.05]	0.67
gly25	FA2G2S2	-0.26 [-1.62:1.11]	0.71
gly29	A3G3S2	0.23 [-1.13:1.59]	0.74
gly31.32	A3G3S3, FA3G3S3	0.20 [-1.01:1.40]	0.75
gly17	M5A1G1S1	-0.19 [-1.52:1.14]	0.78

gly27.28	A3G3S2, A3BG3S2	0.16 [-1.07:1.40]	0.79
gly22	M9	-0.16 [-1.48:1.16]	0.81
gly23	A2G2S2	-0.10 [-1.38:1.17]	0.87
gly12	FA2BG2	-0.07 [-1.46:1.32]	0.92
gly8	A2G2	0.06 [-1.27:1.39]	0.93
gly20.21	A2G2S2	-0.04 [-1.30:1.21]	0.95
gly15	A2G2S1	0.02 [-1.12:1.16]	0.97