

Table S1 Glycosylation precursor synthetic reactions.

Flux No. ^[a]	Reactions
r17	(3) G6P + (6) NADP --> (3) CO2 + (3) R5P + (6) NADPH
r51	G6P --> G1P
r52	G1P + UMPRN + (2) ATP --> UDPG + (2) ADP
r80	UDPG <=> UDPGal
r81	Glc + ATP + GTP --> GDPMann + ADP
r82	F6P + Gln + AcCoA + UTP --> UDPNAG + Glu + CoASH
r83	UDPNAG + ATP + 3PG + CTP --> CMPNeu5Ac + UDP + ADP
r84	GDPMann + NADPH --> GDPFuc + NADP
r85	UDPNAG <=> UDP + GlcNAc
r86	UDPNAG <=> UDPGalNAc
r87	UDPGalNAc <=> GalNAc + UDP
r88	GDPMann <=> Mann + GDP
r89	UDPGal <=> Gal + UDP
r90	CMPNeu5Ac <=> CMP + Neu5Ac
r91	GDPFuc <=> GDP + Fuc
r92	CMPNeu5Ac <=> CMPNeu5Gc
r93	CMPNeu5Gc <=> CMP + Neu5Gc

[a] (The flux ID refers to Sou et al. 2014.)

Table S2 Kinetic model parameters.

Symbol	Explanation	Values	Unit	Reference
Parameters of the Golgi dimension				
	Diameter of the Golgi	7.82 E-5	dm	Del Val, 2011
	Length of the Golgi	0.52 E-5	dm	Del Val, 2011
	Vol μ Me of the Golgi	25 E-15	dm ³	Del Val, 2011
Parameters of the mAb flux (steady state)				
Vol μ Metric	Metric flow rate of N-glycan entering Golgi (ass μ Ming constant)	1.12 E-15	dm ³ min ⁻¹	Del Val, 2011
Parameters of the enzyme concentration (steady state)				
	Enzyme Man I concentration along length z	$3.322 \cdot \exp(-1/2 \cdot ((z-0.255)/(1.57/25))^2)$	μ M	Adjusted from Del Val, 2011
	Enzyme Man II concentration along length z	$4.41 \cdot \exp(-1/2 \cdot ((z-0.388)/(1.15/25))^2)$	μ M	Adjusted from Del Val, 2011
	Enzyme GnTI concentration along length z	$4.114 \cdot \exp(-1/2 \cdot ((z-0.363)/(1.565/25))^2)$	μ M	Adjusted from Del Val, 2011
	Enzyme GnTII concentration along length z	$0.822 \cdot \exp(-1/2 \cdot ((z-0.495)/(1.562/25))^2)$	μ M	Adjusted from Del Val, 2011
	Enzyme GalT concentration along length z	$2 \cdot \exp(-1/2 \cdot ((z-0.525)/(1.506/25))^2)$	μ M	Adjusted from Del Val, 2011
	Enzyme FucT concentration along length z	$1.828 \cdot \exp(-1/2 \cdot ((z-0.776)/(0.9/25))^2)$	μ M	Adjusted from Del Val, 2011
	Enzyme SiaT concentration along length z	$0.164 \cdot \exp(-1/2 \cdot ((z-0.782)/(0.757/25))^2)$	μ M	Adjusted from Del Val, 2011
Parameters of enzymatic kinetic constants				
	Enzyme turnover rate of ManI	888	min ⁻¹	Krambeck and Betenbaugh, 2005
	Enzyme turnover rate of ManII	1924	min ⁻¹	Krambeck and Betenbaugh, 2005
	Enzyme turnover rate of GnTI	1022	min ⁻¹	Krambeck and Betenbaugh, 2005
	Enzyme turnover rate of GnTII	1406	min ⁻¹	Krambeck and Betenbaugh, 2005
	Enzyme turnover rate of GalT	872	min ⁻¹	Krambeck and Betenbaugh, 2005
	Enzyme turnover rate of FucT	291	min ⁻¹	Krambeck and Betenbaugh, 2005
	Enzyme turnover rate of SiaT	491	min ⁻¹	Krambeck and Betenbaugh, 2005
Enzyme dissociation constants (μM)				
	Symbol	Value (del Val, 2011)	Value (Krambeck and Betenbaugh, 2005)	
	KdMAN1OS1 (M9)	60.5 μ M	100 μ M	
	KdMAN1OS2 (M8)	110 μ M	100 μ M	
	KdMAN1OS3 (M7)	30.8 μ M	100 μ M	
	KdMAN1OS4 (M6)	74.1 μ M	100 μ M	
	KdMAN1OS5 (M5)		100 μ M	
	KdMAN2OS6 (M5)	200 μ M	200 μ M	
	KdMAN2OS7 (M4)	100 μ M	200 μ M	
	KdMAN2OS8 (M5)	200 μ M	200 μ M	
	KdMAN2OS10		200 μ M	
	KdMAN2OS12 (M4)		200 μ M	
	KdMAN2OS19		200 μ M	
	KdGNT1OS5	260 μ M	260 μ M	
	KdGNT1OS6	260 μ M	260 μ M	
	KdGNT1GLCNAC	170 μ M	170 μ M	

	KdGNT1UDP	170 μM	170 μM
	KdGNT2OS10	190 μM	190 μM
	KdGNT2OS15	190 μM	190 μM
product)	KdGNT2OS19	190 μM	190 μM
	KdGNT2OS24	190 μM	190 μM
	KdGNT2GLCNAC	960 μM	960 μM
	KdGNT2UDP	960 μM	960 μM
	KdGALTOS6	160 μM	
	KdGALTOS9	160 μM	
	KdGALTOS7	160 μM	
	KdGALTOS8	160 μM	
	KdGALTOS10	160 μM	
	KdGALTOS12	160 μM	
	KdGALTOS19	160 μM	
	KdGALTOS15	160 μM	
product)	KdGALTOS24	160 μM	
	KdGALTOS21	160 μM	
	KdGALTOS28	160 μM	
	KdGALTOS13	160 μM	
	KdGALTOS11	160 μM	
	KdGALTOS18	160 μM	
	KdGALTOS16	6280 μM	
	KdGALTOS25	6280 μM	
	KdGALTOS26	6280 μM	
	KdGALTOS31	6280 μM	
	KdGALTGAL	65 μM	0
	KdGALTUDP	65 μM	0
	KdFUCTOS6	25 μM	25 μM
	KdFUCTOS8	25 μM	25 μM
	KdFUCTOS7	25 μM	25 μM
	KdFUCTOS10	25 μM	25 μM
product)	KdFUCTOS15	25 μM	25 μM
	KdFUCTOS12	25 μM	25 μM
	KdFUCTOS19	25 μM	25 μM
	KdFUCTOS24	25 μM	25 μM
	KdFUCTFUC	46 μM	46 μM
	KdFUCTGDP	46 μM	46 μM
	KdSIATOS9	330 μM	260 μM
	KdSIATOS14	330 μM	260 μM
	KdSIATOS13	330 μM	260 μM
	KdSIATOS11	330 μM	260 μM
	KdSIATOS18	330 μM	260 μM
	KdSIATOS16	330 μM	260 μM
	KdSIATOS25	330 μM	260 μM
	KdSIATOS21	330 μM	260 μM
	KdSIATOS28	330 μM	260 μM
	KdSIATOS26	330 μM	260 μM
product)	KdSIATOS31	330 μM	260 μM
	KdSIATOS30	330 μM	260 μM
	KdSIATOS34	330 μM	260 μM
	KdSIATOS20	330 μM	260 μM
	KdSIATOS17	330 μM	260 μM
	KdSIATOS22	330 μM	260 μM
	KdSIATOS23	330 μM	260 μM
	KdSIATOS27	330 μM	260 μM
	KdSIATOS32	330 μM	260 μM
	KdSIATOS33	330 μM	260 μM
	KdSIATOS35	330 μM	260 μM
	KdSIATSA	50 μM	57 μM
	KdSIATCMP	50 μM	57 μM

Figure S1 Model-simulated glycan profiles in response to variation in each of the four nucleotide sugars.

	Standard - calibrated (μM)	Low concentration boundary - 5 times lower (μM)	High concentration boundary - 5 times higher (μM)
UDP-Gal	9.4	1.9	47
UDP-GlcNAc	1600	320	8000
GDP-Fucose	576	115	2880
CMP-SA	950	190	4750

