Supplementary Information

SI Glycosylation flux analysis of immunoglobulin G in Chinese hamster ovary perfusion cell culture

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Table S1. Summary of the reactor set points and the corresponding measured values.

Experiment	Time [d]	VCD set-point [10^6 cells/d]	PR set-point [reactor volume/d]	VCD [10^6 cells/d]	PR [reactor volume/d]
A	1 – 9	20	1	19.94±0.69	1.01±0.17
	10 – 15	20	0.67	19.82±0.23	0.68±0.03
B	1 – 9	20	1	19.79±0.54	1.14±0.30
	10 – 18	20	2	20.06±0.22	1.93±0.11
C	1 – 12	20	1	19.94±0.40	1.05±0.07
	13 – 21	40	2	39.56±0.45	1.98±0.08
	22 – 28	30	1.5	29.97±0.66	1.49±0.04
D	1 – 9	30	1	30.15±0.42	0.99±0.09
	10 – 19	10	1	10.18±0.12	0.96±0.08
	20 – 27	20	1	20.03±0.33	1.03±0.03

Table S2. Glycan structures in glycosylation network

Glycan Label	**Glycan Structures**
M9	$Man_9GlcNAc_2$
M8	$Man_8GlcNAc_2$
M7	$Man_7GlcNAc_2$
M6	$Man_6GlcNAc_2$
M5	$Man_5GlcNAc_2$
AM5	$GlcNAcMan_5GlcNAc_2$
FAM5	$GlcNAcMan_5GlcNAc_2Fuc$
A1	$GlcNAcMan_3GlcNAc_2$
A2	$GlcNAc_2Man_3GlcNAc_2$
FA1	$GlcNAcMan_3GlcNAc_2Fuc$
FA2	$GlcNAc_2Man_3GlcNAc_2Fuc$
FA1G1	$GalGlcNAcMan_3GlcNAc_2Fuc$
FA2G1-1	$\alpha(1\text{-}6)GalGlcNAc_2Man_3GlcNAc_2Fuc$
FA2G1-2	$\alpha(1\text{-}3)GalGlcNAc_2Man_3GlcNAc_2Fuc$
FA2G2	$Gal_2GlcNAc_2Man_3GlcNAc_2Fuc$
FA2G1-1S1	$\alpha(1\text{-}6)SiaGalGlcNAc_2Man_3GlcNAc_2Fuc$
FA2G1-2S1	$\alpha(1\text{-}3)SiaGalGlcNAc_2Man_3GlcNAc_2Fuc$
FA2G2S1-1	$\alpha(1\text{-}6)SiaGal_2GlcNAc_2Man_3GlcNAc_2Fuc$
FA2G2S1-2	$\alpha(1\text{-}3)SiaGal_2GlcNAc_2Man_3GlcNAc_2Fuc$
FA2G2S2	$Sia_2Gal_2GlcNAc_2Man_3GlcNAc_2Fuc$

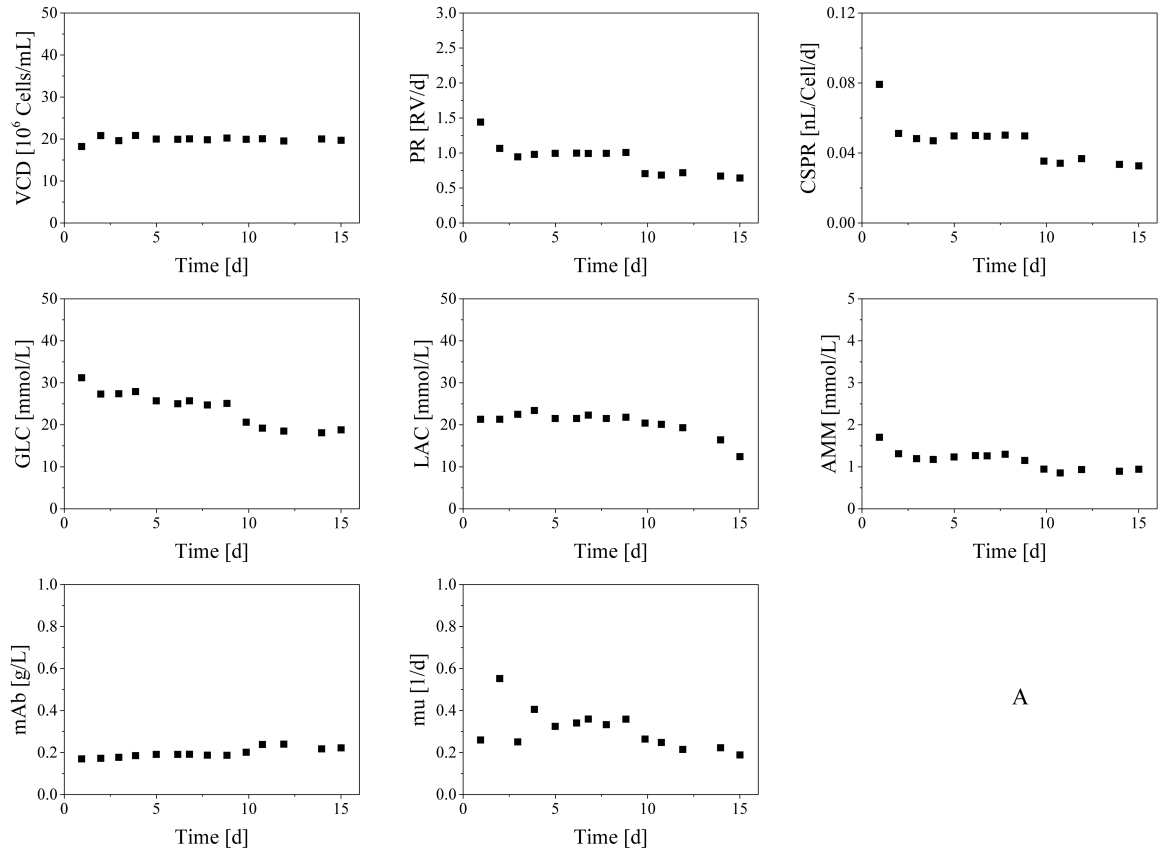

Figure S1. Process measurements in Experiment A.

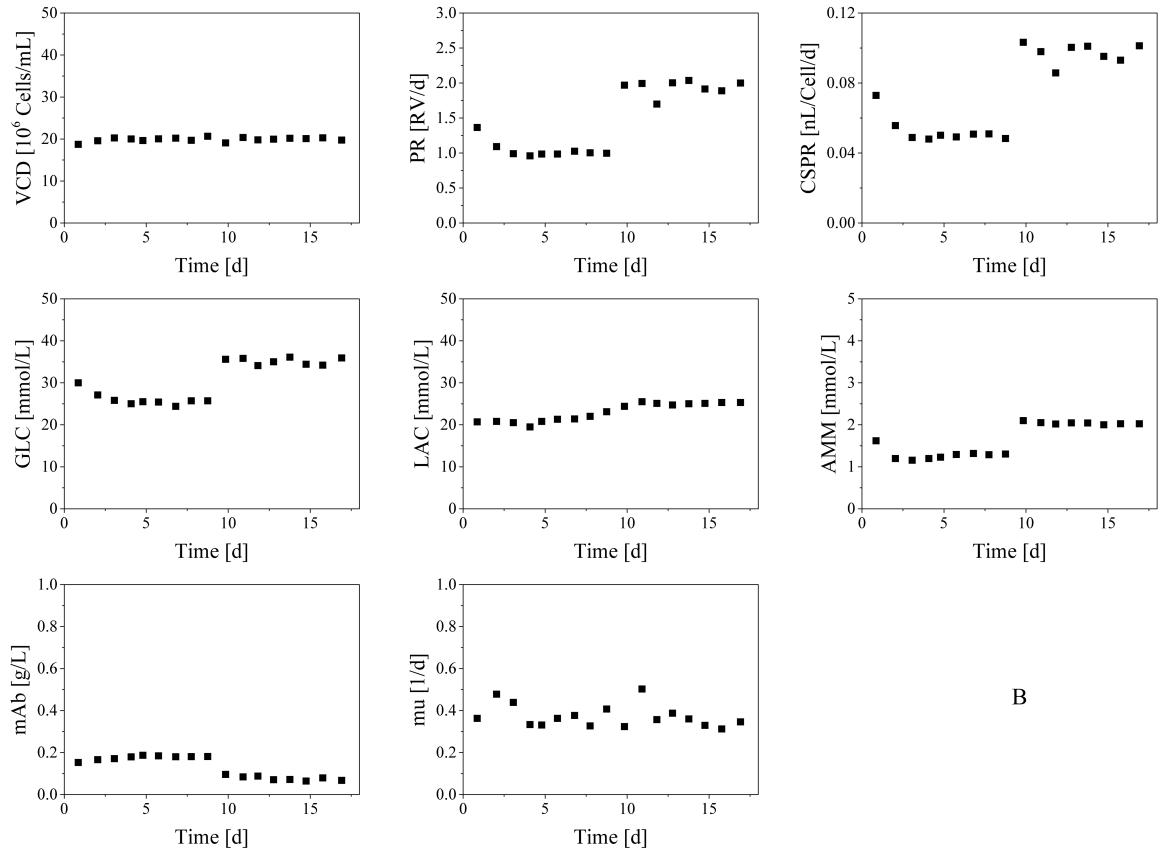

Figure S2. Process measurements in Experiment B.

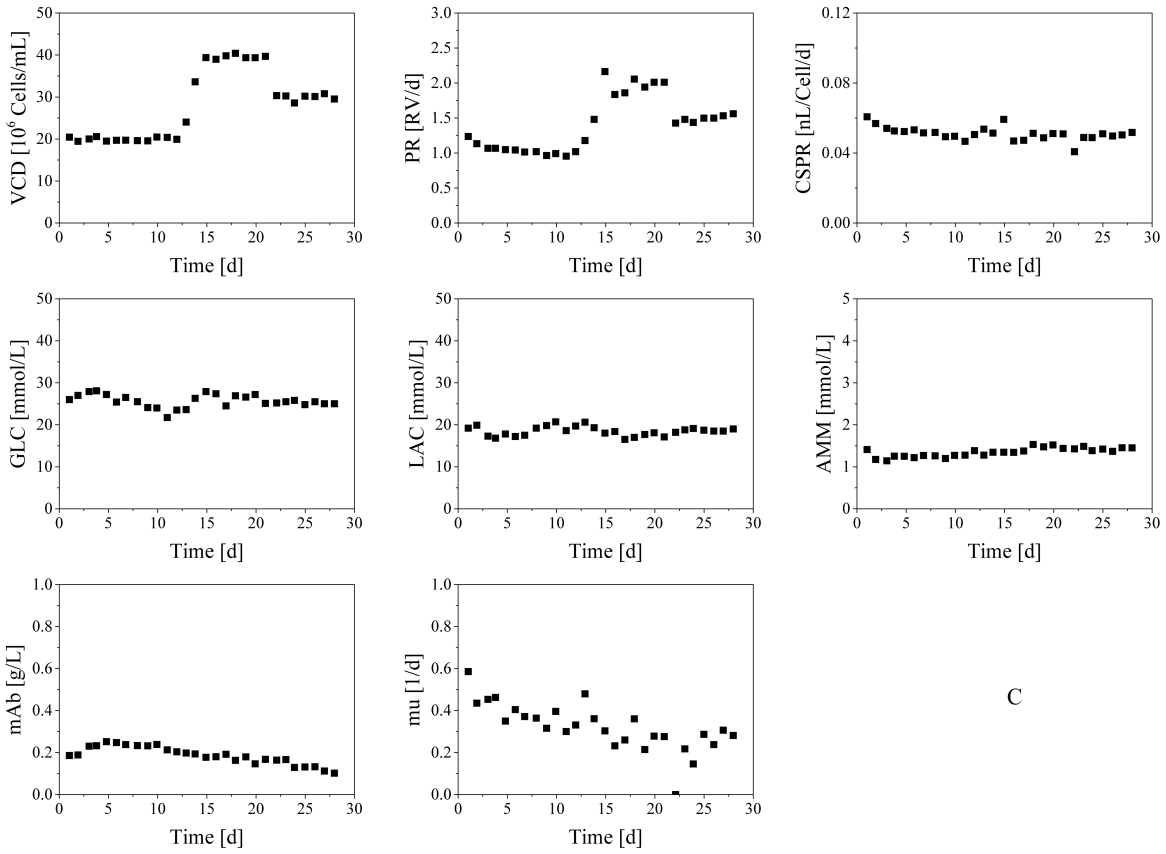

Figure S3. Process measurements in Experiment C.

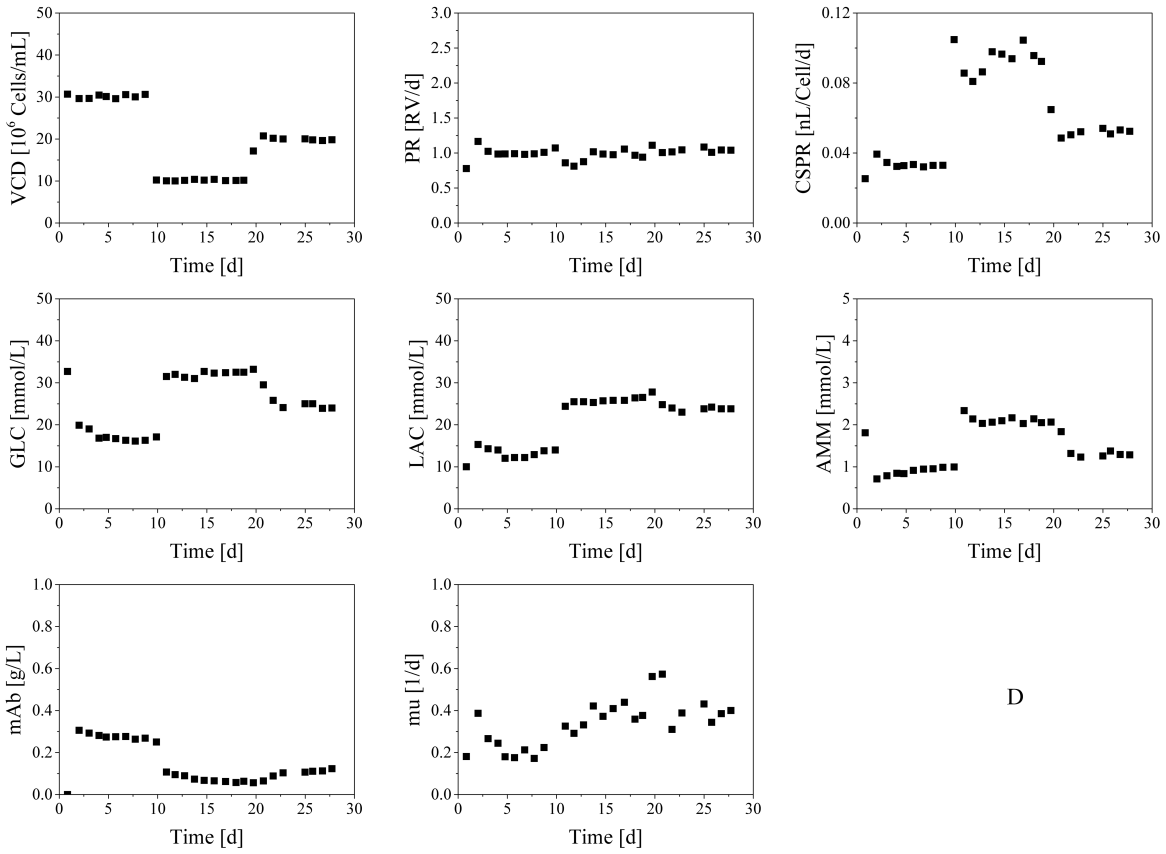

Figure S4. Process measurements in Experiment D.

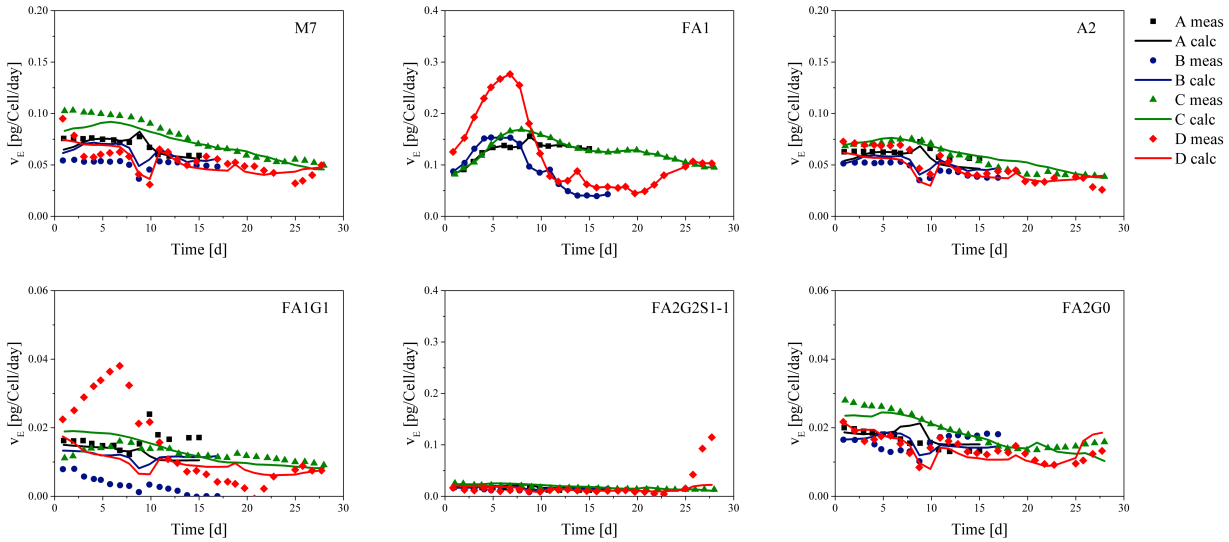

Figure S5. Secretion flux fitting of IgG glycoforms. The solid symbols show the experimental secretion fluxes computed in the data preprocessing step, as outlined in Section 2.2 (Experiment A: black squares, Experiment B: blue circles, Experiment C: green triangle, Experiment D: red diamonds). The lines show the secretion fluxes from the fitting of α_J in the GFA, as outlined in Section 2.3.

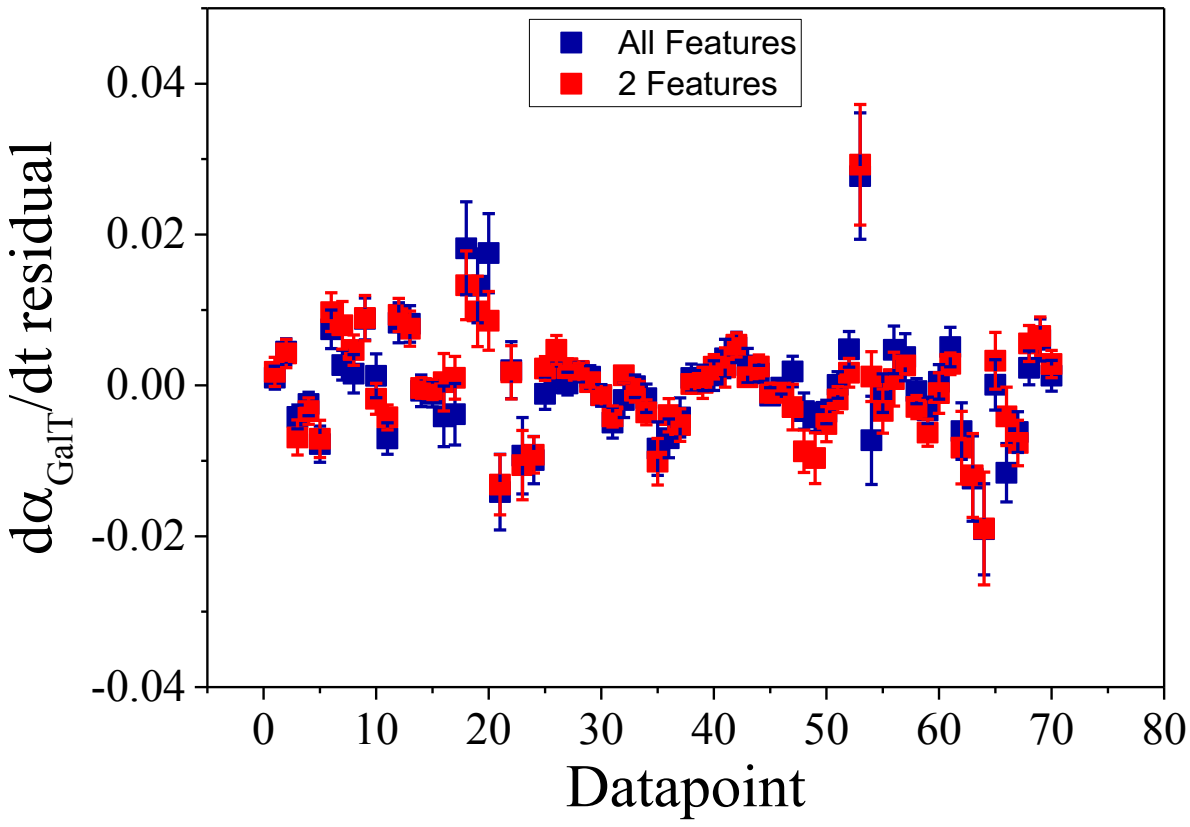

Figure S6. Residuals of random forest regression. Residuals from RF analysis using all features are shown in blue, and those using only cell-specific productivity of IgG q_{IgG} and ammonia concentrations (Amm) are shown in red. The mean and 95% confidence interval were calculated based on 100 repeated runs of random forest regression analysis.