Supplementary Information

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

Sandro Hutter[1,2,a], Moritz Wolf[1,a], Nan Papili Gao[1,2], Dario Lepori[1], Thea Schweigler[1], Massimo Morbidelli[1] and Rudiyanto Gunawan[1,2,3,*]

[1] Institute for Chemical and Bioengineering, Department of Chemistry and Applied Biosciences, ETH Zurich, Zurich 8093, Switzerland
[2] Swiss Institute of Bioinformatics, Lausanne 1015, Switzerland
[3] Department of Chemical and Biological Engineering, University at Buffalo, The State University of New York, Amherst, NY 14260, USA
[a] Contributed equally
* Correspondence: rudiyant@buffalo.edu

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	9-Jan	20	1	19.94±0.69	1.01±0.17
	15-Oct	20	0.67	19.82±0.23	0.68±0.03
B	9-Jan	20	1	19.79±0.54	1.14±0.30
	18-Oct	20	2	20.06±0.22	1.93±0.11
C	12-Jan	20	1	19.94±0.40	1.05±0.07
	15 - 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	9-Jan	30	1	30.15±0.42	0.99±0.09
	19-Oct	10	1	10.18±0.12	0.96±0.08
	21 - 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	$Sia_2Gal_2GlcNAc_2Man_3GlcNAc_2Fuc$

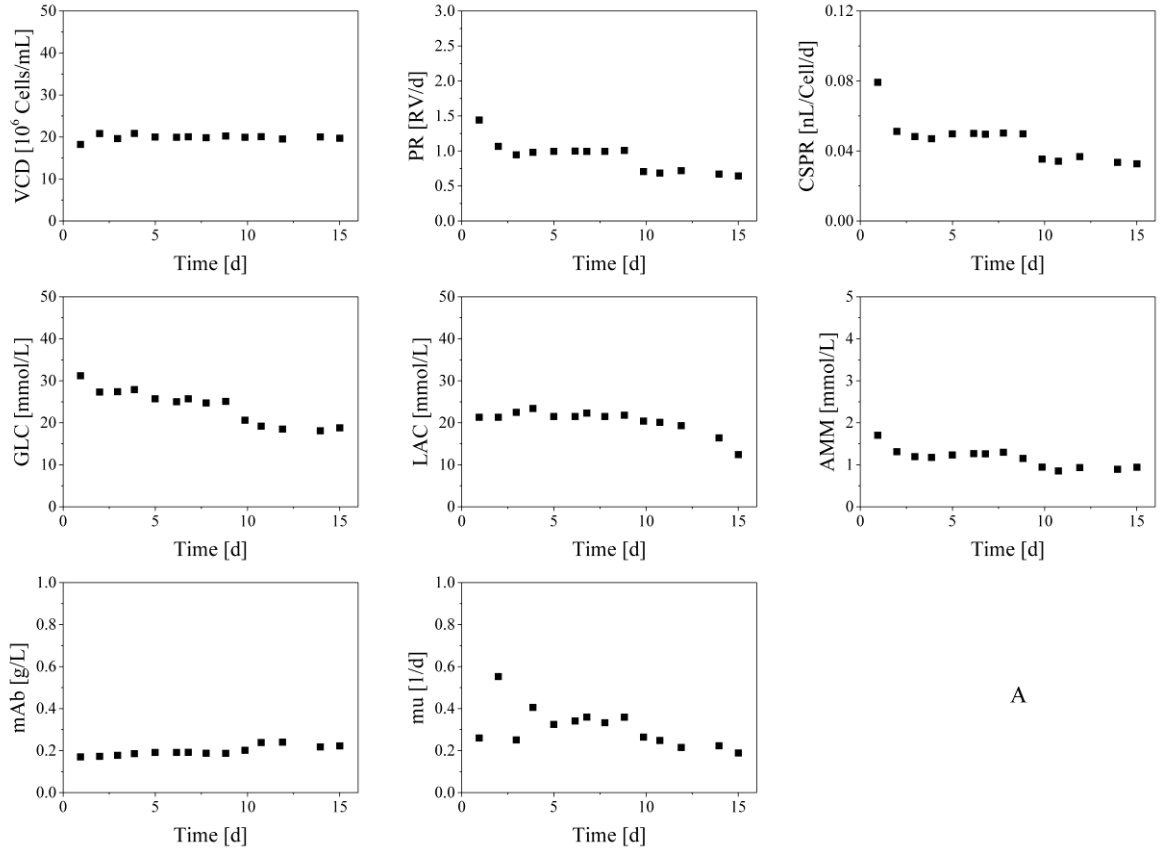

Figure S1. Process measurements in Experiment A.

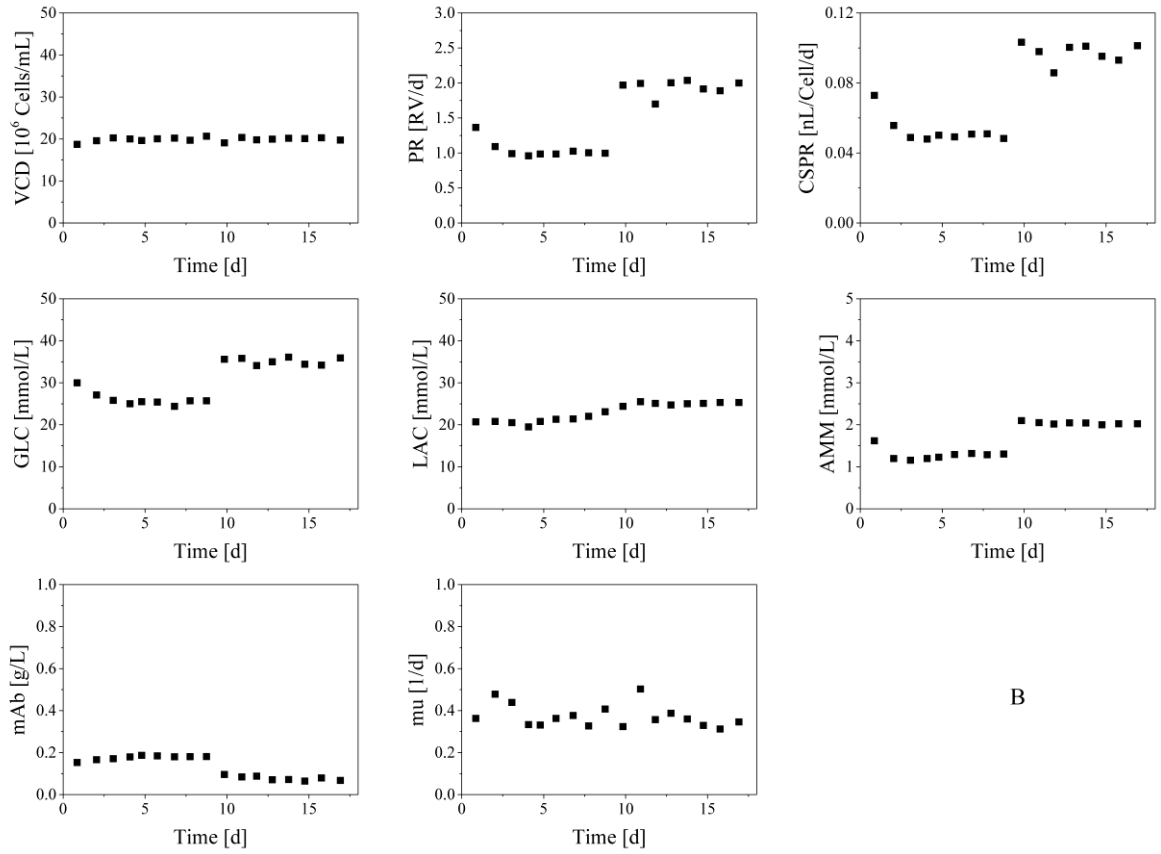

Figure S2. Process measurements in Experiment B.

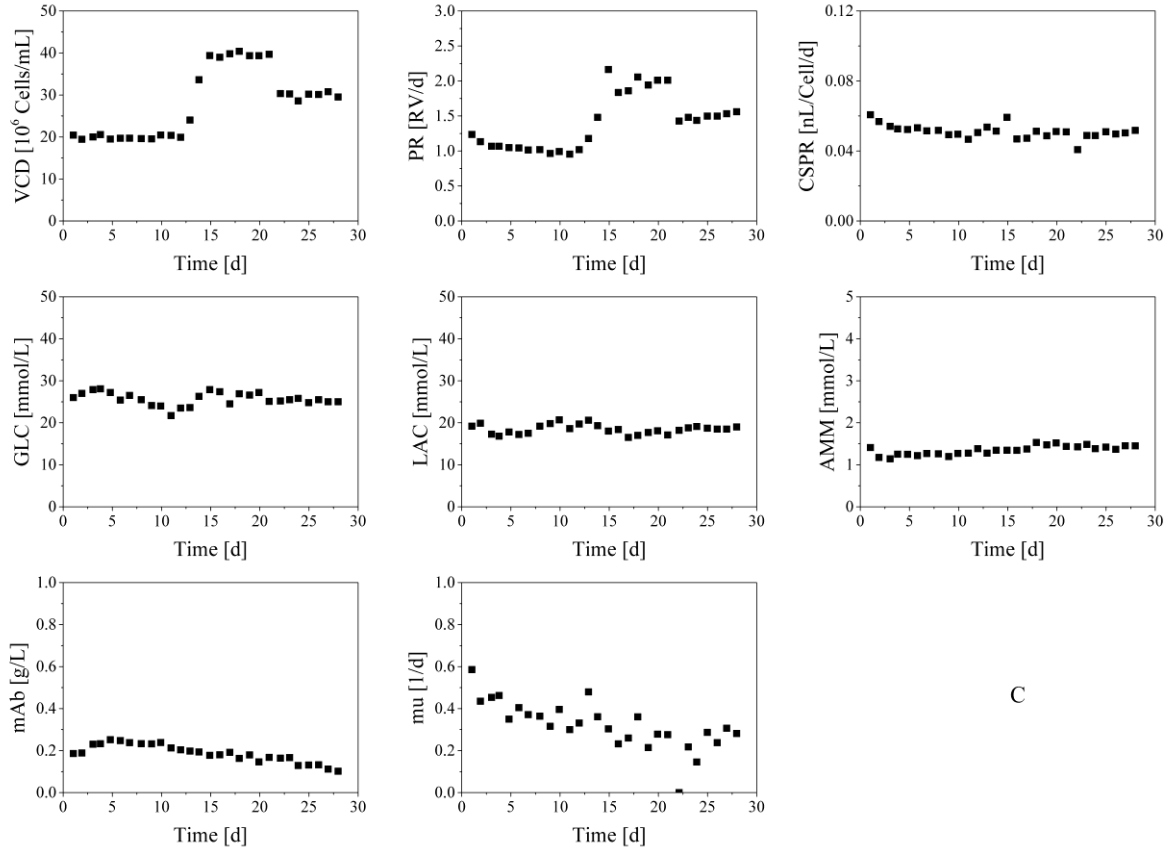

Figure S3. Process measurements in Experiment C.

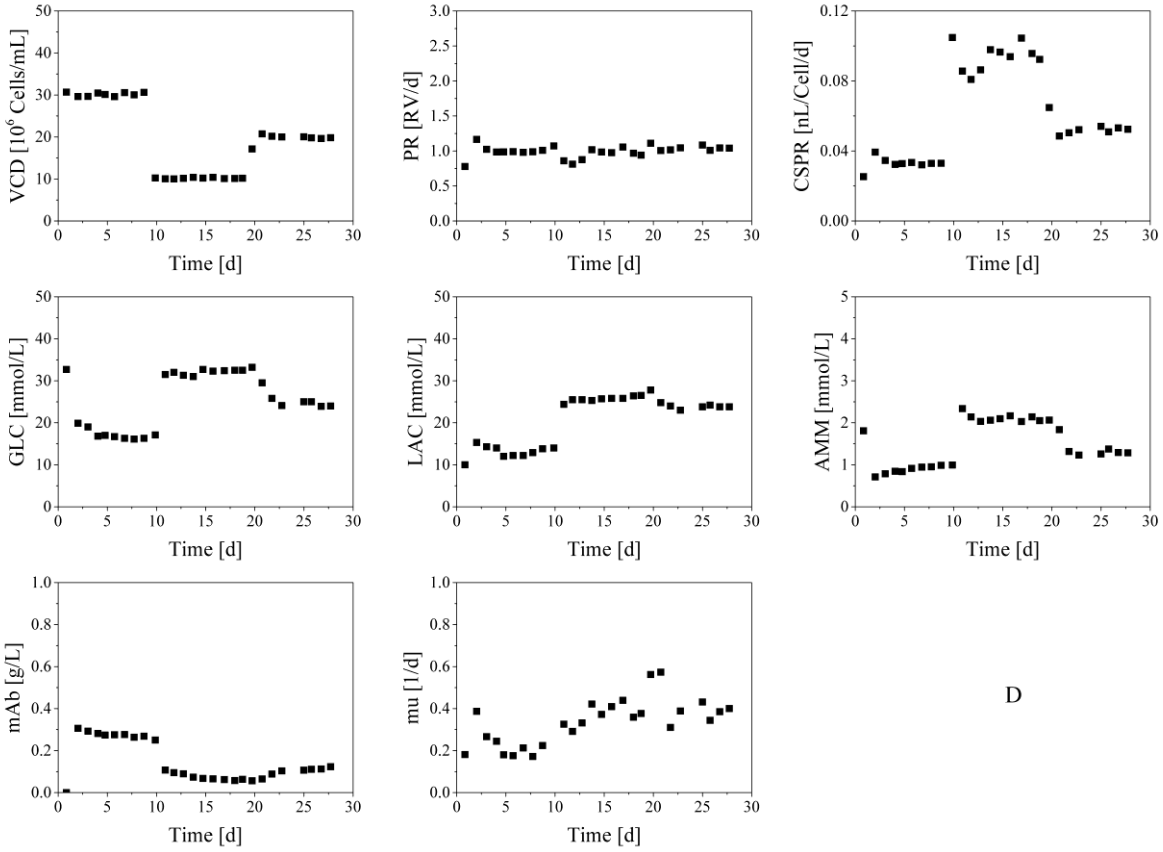

Figure S4. Process measurements in Experiment D.

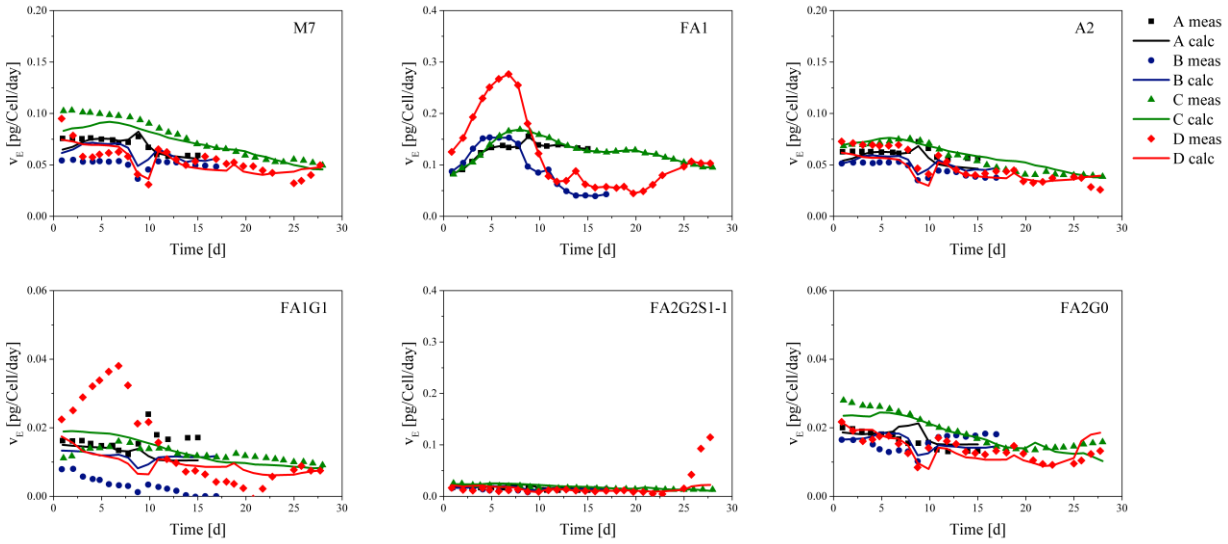

Figure S5. Secretion flux fitting of IgG glycoforms. The solid symbols represent the measured secretion fluxes (Experiment A: black squares, Experiment B: blue circles, Experiment C: green triangle, Experiment D: red diamonds) and the empty symbols show the secretion fluxes predicted by GFA.

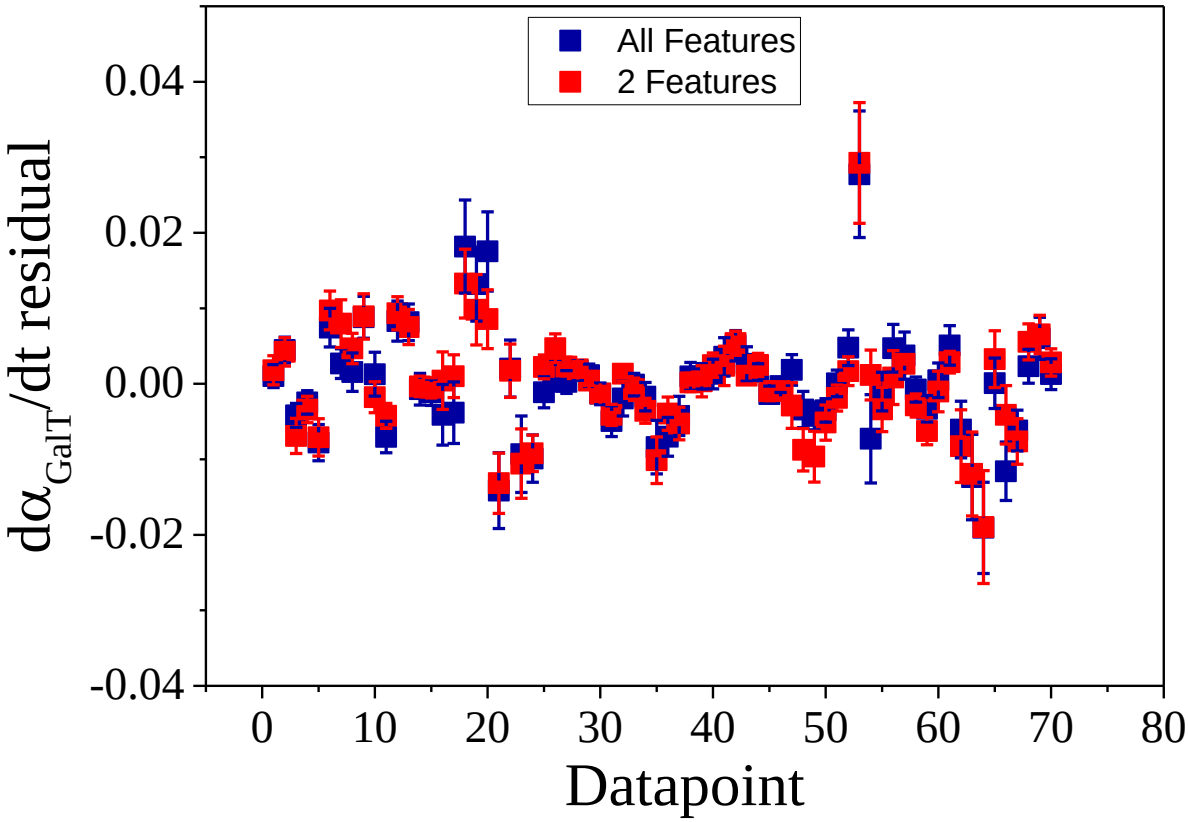

Figure S6. Residuals of random forest regression. Residuals from RF analysis using all features are shown in blue, and those using only cell-specific productivity of IgG q_{IgG} and ammonia concentrations (Amm) are shown in red. The mean and 95% confidence interval were calculated based on 100 repeated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