

Table S1: Total flux intake

flux	D0, D15, D30 (mmol/day)	D45, D60 (mmol/day)	D75, D105 (mmol/day)
EX_5mthf(e)	3.47E-04	2.16E-04	2.09E-04
EX_ala_D(e)	2.33E+01	1.34E+01	1.29E+01
EX_ala_L(e)	2.36E+01	1.37E+01	1.31E+01
EX_arach(e)	2.15E-01	1.97E-01	1.94E-01
EX_arg_L(e)	3.72E+01	2.15E+01	2.07E+01
EX_ascb_L(e)	1.18E+00	7.90E-01	7.67E-01
EX_asp_D(e)	3.32E+01	1.92E+01	1.84E+01
EX_asp_L(e)	3.34E+01	1.93E+01	1.85E+01
EX_avite1(e)	1.86E-02	1.26E-02	1.22E-02
EX_ca2(e)	1.33E+01	8.17E+00	7.88E+00
EX_caro(e)	2.25E-04	1.30E-04	1.25E-04
EX_CE2510(e)	7.41E+00	4.34E+00	4.17E+00
EX_chol(e)	1.43E+00	8.27E-01	7.94E-01
EX_cellul(e)	5.93E-02	3.43E-02	3.29E-02
EX_cu2(e)	6.55E-02	3.86E-02	3.71E-02
EX_cys_L(e)	2.63E-02	1.52E-02	1.46E-02
EX_dca(e)	1.95E-02	1.13E-02	1.08E-02
EX_ddca(e)	2.23E-01	1.29E-01	1.24E-01
EX_doco13ac(e)	5.77E-02	3.33E-02	3.20E-02
EX_docosac(e)	6.14E-02	5.62E-02	5.55E-02
EX_fe2(e)	4.54E-01	2.67E-01	2.57E-01
EX_fe3(e)	2.47E-01	1.47E-01	1.41E-01
EX_fol(e)	4.43E-04	2.72E-04	2.62E-04
EX_fru(e)	6.67E+01	3.86E+01	3.70E+01
EX_glc_D(e)	6.03E+01	3.48E+01	3.35E+01
EX_glu_L(e)	1.08E+02	6.27E+01	6.02E+01
EX_gly(e)	5.57E+01	3.22E+01	3.09E+01
EX_h2o(e)	2.60E+04	1.61E+04	1.56E+04
EX_hdca(e)	3.86E+01	2.47E+01	2.39E+01
EX_hdcea(e)	1.42E+00	1.09E+00	1.07E+00
EX_his_L(e)	1.36E+01	7.87E+00	7.56E+00
EX_hpdca(e)	2.08E+00	1.21E+00	1.16E+00
EX_ile_L(e)	2.62E+01	1.51E+01	1.45E+01
EX_k(e)	1.17E+02	7.09E+01	6.84E+01
EX_leu_L(e)	4.72E+01	2.73E+01	2.62E+01
EX_lgnc(e)	1.76E+00	1.01E+00	9.74E-01
EX_lnlc(e)	6.63E+01	4.04E+01	3.89E+01
EX_lys_L(e)	2.72E+01	1.57E+01	1.51E+01
EX_malt(e)	2.76E-01	1.60E-01	1.53E-01

EX_met_L(e)	8.31E+00	4.80E+00	4.61E+00
EX_mg2(e)	4.52E+01	2.69E+01	2.59E+01
EX_mn2(e)	6.48E-01	3.76E-01	3.62E-01
EX_na1(e)	1.00E+01	5.90E+00	5.67E+00
EX_nac(e)	5.52E-02	3.29E-02	3.17E-02
EX_ncam(e)	5.52E-02	3.29E-02	3.17E-02
EX_ocdca(e)	7.26E+00	4.57E+00	4.42E+00
EX_ocdcea(e)	1.46E+02	9.80E+01	9.51E+01
EX_octa(e)	4.66E-02	2.69E-02	2.59E-02
EX_phe_L(e)	2.47E+01	1.43E+01	1.37E+01
EX_phyQ(e)	6.31E-05	4.37E-05	4.25E-05
EX_pi(e)	2.76E+01	1.62E+01	1.55E+01
EX_pnto_R(e)	2.88E-02	1.67E-02	1.60E-02
EX_pro_D(e)	1.90E+01	1.10E+01	1.06E+01
EX_pro_L(e)	1.92E+01	1.11E+01	1.07E+01
EX_pydam(e)	3.10E-03	2.14E-03	2.08E-03
EX_pydx(e)	3.14E-03	2.16E-03	2.11E-03
EX_pydxn(e)	3.10E-03	2.14E-03	2.08E-03
EX_ribflv(e)	2.88E-03	1.88E-03	1.82E-03
EX_ser_L(e)	3.95E+01	2.28E+01	2.19E+01
EX_starch1200(e)	7.06E-01	4.08E-01	3.92E-01
EX_strch1(e)	7.38E-01	4.27E-01	4.10E-01
EX_strch2(e)	2.64E+00	1.52E+00	1.46E+00
EX_sucr(e)	1.98E+01	1.14E+01	1.10E+01
EX_thf(e)	3.59E-04	2.23E-04	2.16E-04
EX_thm(e)	9.61E-03	5.70E-03	5.49E-03
EX_thr_L(e)	2.61E+01	1.51E+01	1.45E+01
EX_trp_L(e)	4.54E+00	2.62E+00	2.52E+00
EX_ttdca(e)	3.19E-01	1.84E-01	1.77E-01
EX_tyr_L(e)	1.48E+01	8.54E+00	8.20E+00
EX_val_L(e)	3.61E+01	2.09E+01	2.01E+01
EX_zn2(e)	3.37E-01	1.96E-01	1.88E-01
EX_HC00229(e)	2.26E+01	2.31E+01	6.88E+01
EX_dextrin(e)	1.87E+01	1.91E+01	5.70E+01
EX_kesto(e)	3.06E+00	3.13E+00	9.33E+00
EX_kestopt(e)	1.86E+00	1.91E+00	5.68E+00
EX_kestottr(e)	2.32E+00	2.37E+00	7.06E+00

Table S2: Manually added flux for adlay

metabolites in flux	adlay composition (g metabolites/100g adlay)	D0, D15, D30 (mmol/day)	D45, D60 (mmol/day)	D75, D105 (mmol/day)
EX_etoh[e]		0.00E+00	0.00E+00	0.00E+00
EX_h2o[e]	8.79E+00	1.09E+03	6.28E+02	6.03E+02
EX_caro[e]		0.00E+00	0.00E+00	0.00E+00
EX_retinol[e]		0.00E+00	0.00E+00	0.00E+00
EX_thm[e]	2.00E-05	1.68E-04	9.69E-05	9.31E-05
EX_adpcbl[e]		0.00E+00	0.00E+00	0.00E+00
EX_ribflv[e]	5.00E-05	2.96E-04	1.71E-04	1.64E-04
EX_nac[e]		0.00E+00	0.00E+00	0.00E+00
EX_ncam[e]		0.00E+00	0.00E+00	0.00E+00
EX_pnto_R[e]	5.00E-04	5.10E-03	2.95E-03	2.83E-03
EX_pydam[e]		0.00E+00	0.00E+00	0.00E+00
EX_pydxn[e]		0.00E+00	0.00E+00	0.00E+00
EX_pydx[e]		0.00E+00	0.00E+00	0.00E+00
EX_btn[e]		0.00E+00	0.00E+00	0.00E+00
EX_10fthf[e]		0.00E+00	0.00E+00	0.00E+00
EX_5mthf[e]		0.00E+00	0.00E+00	0.00E+00
EX_thf[e]		0.00E+00	0.00E+00	0.00E+00
EX_ascb_L[e]		0.00E+00	0.00E+00	0.00E+00
EX_vitd3[e]		0.00E+00	0.00E+00	0.00E+00
EX_avite1[e]	1.00E-04	5.17E-04	2.99E-04	2.87E-04
EX_phyQ[e]		0.00E+00	0.00E+00	0.00E+00
EX_ca2[e]	1.05E-02	5.85E-01	3.38E-01	3.25E-01
EX_cl[e]		0.00E+00	0.00E+00	0.00E+00
EX_k[e]	2.74E-01	1.56E+01	9.03E+00	8.67E+00
EX_mg2[e]	1.73E-01	1.58E+01	9.15E+00	8.78E+00
EX_na1[e]	9.00E-03	8.71E-01	5.03E-01	4.83E-01
EX_pi[e]	3.62E-01	8.40E+00	4.85E+00	4.66E+00
EX_cu2[e]	5.39E-04	1.89E-02	1.09E-02	1.05E-02
EX_fe2[e]	5.21E-03	2.08E-01	1.20E-01	1.15E-01
EX_fe3[e]		0.00E+00	0.00E+00	0.00E+00
EX_mn2(e)	2.79E-03	1.13E-01	6.53E-02	6.27E-02
EX_zn2(e)	4.14E-03	1.41E-01	8.15E-02	7.83E-02
EX_mnl(e)		0.00E+00	0.00E+00	0.00E+00
EX_xylt[e]		0.00E+00	0.00E+00	0.00E+00
EX_lcts[e]		0.00E+00	0.00E+00	0.00E+00
EX_malt[e]		0.00E+00	0.00E+00	0.00E+00
EX_sucr[e]		0.00E+00	0.00E+00	0.00E+00

EX_fru[e]		0.00E+00	0.00E+00	0.00E+00
EX_gal[e]		0.00E+00	0.00E+00	0.00E+00
EX_cellul(e)	2.16E+00	5.93E-02	3.43E-02	3.29E-02
EX_ala_L[e]	1.54E-02	3.83E-01	2.22E-01	2.13E-01
EX_arg_L[e]	6.20E-03	7.87E-02	4.55E-02	4.37E-02
EX_asp_L[e]	9.44E-03	1.59E-01	9.19E-02	8.83E-02
EX_cys_L[e]	1.43E-03	2.63E-02	1.52E-02	1.46E-02
EX_glu_L[e]	3.56E-02	5.42E-01	3.13E-01	3.01E-01
EX_gly[e]	3.53E-03	1.05E-01	6.05E-02	5.81E-02
EX_urate[e]	0.00E+00	0.00E+00	0.00E+00	0.00E+00
EX_his_L[e]	4.85E-03	6.96E-02	4.02E-02	3.86E-02
EX_ile_L[e]	5.90E-03	1.00E-01	5.79E-02	5.56E-02
EX_leu_L[e]	2.19E-02	3.71E-01	2.15E-01	2.06E-01
EX_lys_L[e]	2.54E-03	3.84E-02	2.22E-02	2.13E-02
EX_met_L[e]	1.30E-03	1.94E-02	1.12E-02	1.08E-02
EX_phe_L[e]	8.16E-03	1.10E-01	6.35E-02	6.10E-02
EX_pro_L[e]	1.09E-02	2.11E-01	1.22E-01	1.17E-01
EX_ser_L[e]	6.86E-03	1.45E-01	8.40E-02	8.06E-02
EX_thr_L[e]	4.48E-03	8.37E-02	4.84E-02	4.65E-02
EX_trp_L[e]	0.00E+00	0.00E+00	0.00E+00	0.00E+00
EX_tyr_L[e]	6.11E-03	7.50E-02	4.34E-02	4.17E-02
EX_val_L[e]	7.90E-03	1.50E-01	8.67E-02	8.33E-02
EX_dca[e]		0.00E+00	0.00E+00	0.00E+00
EX_ddca[e]		0.00E+00	0.00E+00	0.00E+00
EX_ttdca[e]	4.60E-03	4.50E-02	2.60E-02	2.50E-02
EX_ttdcea[e]		0.00E+00	0.00E+00	0.00E+00
EX_ptdca[e]		0.00E+00	0.00E+00	0.00E+00
EX_hdca[e]	1.12E+00	9.76E+00	5.64E+00	5.42E+00
EX_hpdca[e]	2.50E-01	2.06E+00	1.19E+00	1.15E+00
EX_ocdca[e]	3.60E-01	2.83E+00	1.63E+00	1.57E+00
EX_ocdcea[e]	4.91E+00	3.88E+01	2.24E+01	2.16E+01
EX_lnlc[e]		0.00E+00	0.00E+00	0.00E+00
EX_lnlnc[e]		0.00E+00	0.00E+00	0.00E+00
EX_strdnc[e]		0.00E+00	0.00E+00	0.00E+00
EX_arach[e]		0.00E+00	0.00E+00	0.00E+00
EX_CE2510[e]	8.40E-01	6.04E+00	3.49E+00	3.35E+00
EX_CE4843[e]		0.00E+00	0.00E+00	0.00E+00
EX_arachd[e]		0.00E+00	0.00E+00	0.00E+00
EX_docosac[e]		0.00E+00	0.00E+00	0.00E+00
EX_doco13ac[e]		0.00E+00	0.00E+00	0.00E+00
EX_adrn[e]		0.00E+00	0.00E+00	0.00E+00
EX_clpnd[e]		0.00E+00	0.00E+00	0.00E+00
EX_crvnc[e]		0.00E+00	0.00E+00	0.00E+00
EX_but[e]		0.00E+00	0.00E+00	0.00E+00

EX_octa[e]		0.00E+00	0.00E+00	0.00E+00
EX_chsterol[e]		0.00E+00	0.00E+00	0.00E+00
EX_sbt_D[e]		0.00E+00	0.00E+00	0.00E+00
EX_glc_D[e]		0.00E+00	0.00E+00	0.00E+00
EX_hdcea[e]	5.00E-02	4.39E-01	2.54E-01	2.44E-01
EX_lgnc[e]	2.90E-01	1.76E+00	1.01E+00	9.74E-01
EX_fol[e]	1.60E-05	8.08E-05	4.67E-05	4.49E-05
EX_strch1[e]		0.00E+00	0.00E+00	0.00E+00
EX_i[e]		0.00E+00	0.00E+00	0.00E+00
EX_starch1200(e)	6.12E+01	6.99E-01	4.04E-01	3.88E-01

Table S3: Manually added flux for other nutritions

other metabolites	D0, D15, D30 (mmol/day)	D45, D60 (mmol/day)	D75, D105 (mmol/day)
isomaltose	22.56	23.08	68.77
dxtrin	18.70	19.13	57.01
kestose	3.06	3.13	9.33
kestopentaose	1.86	1.91	5.68
kestotetraose	2.32	2.37	7.06