SUPPLEMENTARY MATERIAL III

Isotopomer abundances of measurements considered during ILE designs

The following tables list the isotopomer abundances of the metabolites (tables 1 and 2) considered during ILE designs of PPP and GABA shunt pathways. The NMR isotopomer abundance measurements were converted to MS-like mass isotopomer abundance measurements because the program NMR2Flux accepts mass isotopomer abundances only. The metabolites on passing through a MS are broken down into fragments. We numbered the C atoms in the metabolites according to IUPAC nomenclature. The fragments are represented by the number of the C atom from the original molecule present in it. The number of mass isotopomer measurements for a fragment obtained from MS = 1+ No. of C atoms in fragment. This number varies for fragments obtained from NMR depending on the Jcc coupling between adjacent carbon atoms.

Mass isotopomers included in the PPP network

Metabolite measured	Fragment	# of Mass isotopomer measurements	Metabolic precursor
Ala_m	23	3	T3P
	123	4	
Gly_m	2	2	T3Pp
	12	3	
Val_m	12	3	T3Pp
	2345	5	
	12345	6	
Ser_m	12	3	T3Pp
	23	3	
	123	4	
His_m	2345	5	P5Pp
Phe_m	12	3	T3Pp, E4Pp
	23456789	9	
	123456789	10	
Tyr_m	12	3	T3Pp, E4Pp
	23456789	9	
	123456789	10	
ribose	12	3	
	345	4	P5P
	2345	5	
	12345	6	
starch	56	2	G6Pp

	456	4	
	1234	5	
	3456	5	
	12345	6	
	123456	7	
glucose	56	2	G6P
	456	4	
	1234	5	
	3456	5	
	12345	6	
	123456	7	
Ala_n	2	2	T3P
	3	2	
	12	1	
	23	2	
	123	1	
Ser_n	2	2	T3Pp
	3	2	
	23	1	
Val_n	2	2	T3Pp
	3	2	
	4	2	
	5	2	
	34	1	
	35	1	
His_n	1	2	P5Pp
	3	2	
	4	2	
	12	1	
	23	1	
	34	2	
	45	1	
	234	1	
	345	1	
Tyr_n	2	2	T3Pp
	3	2	
	12	1	
	23	1	
	34	1	
	234	1	
	123	1	
Phe_n	2	2	T3Pp, E4Pp
	3	2	
	7	2	
	12	1	
	23	1	
	34	1	
	67	1	
	78	1	
	123	1	
	234	1	
	678	1	
LVgc	3	2	G6P
	4	2	
	6	2	
	23	1	

Metabolite	Fragment	#	Metabolic precursor
	34	2	
	45	1	
	56	1	
	234	1	
	456	1	
	3456	1	
LVgp	3	2	G6Pp
	4	2	
	6	2	
	23	1	
	34	2	
	45	1	
	56	1	
	234	1	
	456	1	
	3456	1	
LVrc	2	2	P5P
	3	2	
	5	2	
	12	1	
	23	2	
	34	1	
	45	1	
	123	1	
	345	1	
	2345	1	
Gly_n	12	1	T3Pp

Mass isotopomers included in the GABA shunt network

Metabolite measured	Fragment	# of Mass isotopomer measurements	Metabolic precursor
Ala_m	23	3	pyr_m
	123	4	
Gly_m	2	2	pyr_c
	12	3	
Val_m	12	3	pyr_m
	23	3	
	123	4	
Leu_m	12	3	ACA_m, pyr_m
	23456	6	
Ile_m	12	3	OAA_m, pyr_m
	23456	6	
pro_m	2345	5	$2OG_m$
	12345	6	
Ser_m	12	3	pyr_c
	23	3	
	123	4	
Thr_m	234	4	OAA_m

	1234	5	
Asp_m	12	3	OAA_m
	234	4	
	1234	5	
Glu_m	2345	5	$2OG_m$
	12345	6	
Lys_m	12	3	$2OG_m$, ACA_m
	23456	6	
	123456	7	
Arg_m	2345	5	$2OG_m$
	12345	6	
Ala_n	2	2	pyr_m
	3	2	
	12	1	
	23	2	
	123	1	
Arg_n	2	2	$2OG_m$
	3	2	
	4	2	
	5	2	
	23	1	
	34	1	
	45	1	
	234	1	
Asp_n	2	2	OAA_m
	3	2	
	12	1	
	23	1	
	34	1	
	123	1	
	234	1	
Glu_n	2	2	$2OG_m$
	3	2	
	4	2	
	34	1	
	45	1	
	345	1	
Met_n	2	2	OAA_m
	3	2	
	4	2	
	12	1	
	123	1	
Pro_n	2	2	$2OG_m$
	3	2	
	4	2	
	5	2	
	45	2	
	345	1	

Ser_n	2	2	pyr_c
	3	2	
	23	1	
Thr_n	2	2	OAA_m
	3	2	
	4	2	
	12	1	
	23	2	
	34	2	
	123	1	
	234	1	
Ile_n	3	2	OAA_m, pyr_m
	4	2	
	5	2	
	6	2	
	34	1	
	36	1	
	45	1	
	345	1	
Leu_n	2	2	ACA_m, pyr_m
	3	2	
	4	2	
	5	2	
	6	2	
	12	1	
	23	1	
	45	1	
	123	1	
Lys_n	2	2	$2OG_m$, ACA_m
	3	2	
	4	2	
	5	2	
	6	2	
	23	1	
	34	1	
	45	1	
	234	1	
	345	1	
Val_n	2	2	pyr_m
	3	2	
	4	2	
	5	2	
	34	1	
	35	1	