Electronic Supplementary Material (ESI) for Molecular BioSystems

Supplementary Tables

Table S1. Isotopomer abundances of proteinogenic amino acids from poplar cell suspensions grown under light for 7 d.

Fragments (↓) | Labels (→)				28% U-13C					100% 1-13C					98% U-13C				
AA	frag	MW-frag	n(m+n)	Rep 1	Rep 2	Rep 3	Avg	SD	Rep 1	Rep 2	Rep 3	Avg	SD	Rep 1	Rep 2	Rep 3	Avg	SD
Ala	[23]	232	0	66%	66%	66%	66%	0%	63%	64%	63%	63%	0%	ND	ND	ND	ND	ND
Ala	[23]	232	1	10%	11%	10%	11%	0%	36%	35%	35%	35%	0%	ND	ND	ND	ND	ND
Ala	[23]	232	2	23%	23%	23%	23%	0%	1%	1%	1%	1%	0%	ND	ND	ND	ND	ND
Ala	[123]	260	0	61%	60%	61%	61%	0%	61%	61%	61%	61%	0%	3%	3%	4%	3%	0%
Ala	[123]	260	1	13%	13%	13%	13%	0%	37%	36%	37%	37%	0%	2%	2%	2%	2%	0%
Ala	[123]	260	2	8%	8%	8%	8%	0%	3%	3%	3%	3%	0%	2%	2%	2%	2%	0%
Ala	[123]	260	3	19%	18%	18%	18%	0%	0%	0%	0%	0%	0%	93%	93%	93%	93%	0%
Asp	[12]	302	0	65%	66%	65%	65%	0%	73%	72%	72%	72%	0%	11%	10%	11%	11%	0%
Asp	[12]	302	1	19%	19%	19%	19%	0%	25%	26%	26%	26%	0%	9%	9%	9%	9%	0%
Asp	[12]	302	2	16%	16%	16%	16%	0%	2%	2%	2%	2%	0%	80%	81%	81%	81%	0%
Asp	[234]	316	0	54%	54%	54%	54%	0%	55%	55%	55%	55%	0%	7%	7%	7%	7%	0%
Asp	[234]	316	1	23%	24%	23%	23%	0%	37%	37%	37%	37%	0%	6%	6%	6%	6%	0%
Asp	[234]	316	2	15%	15%	15%	15%	0%	7%	7%	7%	7%	0%	12%	12%	12%	12%	0%
Asp	[234]	316	3	7%	7%	8%	7%	0%	1%	1%	1%	1%	0%	75%	76%	75%	75%	0%
Asp	[234]	390	0	54%	55%	55%	55%	0%	56%	56%	56%	56%	0%	7%	7%	7%	7%	0%
Asp	[234]	390	1	23%	23%	23%	23%	0%	36%	37%	37%	37%	0%	6%	5%	6%	6%	0%
Asp	[234]	390	2	15%	15%	15%	15%	0%	7%	7%	7%	7%	0%	12%	12%	12%	12%	0%
Asp	[234]	390	3	7%	7%	7%	7%	0%	0%	0%	0%	0%	0%	75%	76%	75%	75%	0%
Asp	[1234]	418	0	48%	47%	47%	47%	0%	49%	48%	48%	49%	1%	6%	6%	6%	6%	0%
Asp	[1234]	418	1	22%	22%	22%	22%	0%	39%	40%	40%	39%	0%	3%	3%	3%	3%	0%
Asp	[1234]	418	2	17%	17%	17%	17%	0%	11%	11%	11%	11%	0%	7%	7%	7%	7%	0%
Asp	[1234]	418	3	10%	10%	11%	10%	0%	1%	1%	1%	1%	0%	13%	12%	13%	13%	1%
Asp	[1234]	418	4	3%	3%	3%	3%	0%	0%	0%	0%	0%	0%	70%	72%	70%	71%	1%
Glu	[2345]	272	0	40%	40%	40%	40%	0%	39%	39%	39%	39%	0%	1%	1%	1%	1%	0%
Glu	[2345]	272	1	23%	24%	24%	24%	0%	43%	43%	43%	43%	0%	2%	1%	2%	2%	0%
Glu	[2345]	272	2	25%	25%	25%	25%	0%	16%	16%	16%	16%	0%	5%	5%	5%	5%	0%
Glu	[2345]	272	3	8%	8%	8%	8%	0%	2%	2%	2%	2%	0%	10%	10%	10%	10%	0%
Glu	[2345]	272	4	4%	4%	4%	4%	0%	0%	0%	0%	0%	0%	82%	82%	82%	82%	0%
Glu	[2345]	330	0	41%	41%	41%	41%	0%	40%	39%	39%	39%	0%	2%	2%	2%	2%	0%
Glu	[2345]	330	1	23%	24%	23%	23%	0%	43%	43%	43%	43%	0%	2%	1%	2%	2%	0%
Glu	[2345]	330	2	25%	25%	25%	25%	0%	15%	16%	16%	16%	0%	6%	6%	6%	6%	0%
Glu	[2345]	330	3	7%	7%	7%	7%	0%	2%	2%	2%	2%	0%	9%	9%	9%	9%	0%
Glu	[2345]	330	4	3%	3%	3%	3%	0%	0%	0%	0%	0%	0%	82%	83%	82%	82%	0%
Glu	[12345]	432	0	35%	35%	35%	35%	0%	35%	34%	34%	34%	1%	1%	1%	1%	1%	0%
Glu	[12345]	432	1	21%	22%	22%	22%	0%	43%	43%	43%	43%	0%	1%	1%	1%	1%	0%
Glu	[12345]	432	2	25%	25%	25%	25%	0%	18%	19%	19%	19%	0%	2%	2%	2%	2%	0%
Glu	[12345]	432	3	13%	13%	13%	13%	0%	3%	4%	4%	4%	0%	6%	6%	7%	6%	0%
Glu	[12345]	432	4	5%	5%	4%	5%	0%	0%	0%	0%	0%	0%	11%	11%	12%	11%	0%
Glu	[12345]	432	5	2%	2%	2%	2%	0%	0%	0%	0%	0%	0%	78%	78%	77%	78%	1%
Gly	[2]	218	0	73%	73%	73%	73%	0%	ND	ND	ND	ND	ND	11%	11%	11%	11%	0%

Supplementary Tables

Table S1. Isotopomer abundances of proteinogenic amino acids from poplar cell suspensions grown under light for 7 d.

Fragments (↓) | Labels (→)				28% U-13C					100% 1-13C					98% U-13C				
AA	frag	MW-frag	n(m+n)	Rep 1	Rep 2	Rep 3	Avg	SD	Rep 1	Rep 2	Rep 3	Avg	SD	Rep 1	Rep 2	Rep 3	Avg	SD
Gly	[2]	218	1	27%	27%	27%	27%	0%	ND	ND	ND	ND	ND	89%	89%	89%	89%	0%
Gly	[12]	246	0	64%	63%	64%	64%	0%	92%	91%	91%	91%	1%	7%	7%	7%	7%	0%
Gly	[12]	246	1	18%	18%	17%	18%	0%	8%	9%	9%	9%	0%	5%	4%	5%	5%	0%
Gly	[12]	246	2	18%	19%	19%	19%	0%	0%	1%	1%	0%	0%	88%	89%	88%	88%	0%
His	[2345]	196	0	36%	36%	35%	36%	1%	58%	58%	57%	58%	0%	9%	8%	8%	8%	0%
His	[2345]	196	1	31%	32%	32%	32%	1%	34%	34%	34%	34%	0%	1%	1%	1%	1%	0%
His	[2345]	196	2	20%	20%	20%	20%	0%	7%	7%	7%	7%	0%	1%	2%	2%	2%	0%
His	[2345]	196	3	10%	10%	10%	10%	0%	1%	1%	1%	1%	0%	12%	13%	12%	12%	0%
His	[2345]	196	4	2%	2%	2%	2%	0%	0%	0%	1%	1%	0%	77%	76%	76%	76%	0%
Ile	[23456]	200	0	45%	45%	45%	45%	0%	45%	44%	44%	44%	0%	ND	ND	ND	ND	ND
Ile	[23456]	200	1	18%	18%	18%	18%	0%	38%	38%	38%	38%	0%	ND	ND	ND	ND	ND
Ile	[23456]	200	2	22%	22%	22%	22%	0%	15%	15%	15%	15%	0%	ND	ND	ND	ND	ND
Ile	[23456]	200	3	10%	10%	10%	10%	0%	2%	2%	2%	2%	0%	ND	ND	ND	ND	ND
Ile	[23456]	200	4	3%	3%	3%	3%	0%	0%	0%	0%	0%	0%	ND	ND	ND	ND	ND
Ile	[23456]	200	5	2%	1%	1%	2%	0%	0%	0%	0%	0%	0%	ND	ND	ND	ND	ND
Leu	[23456]	200	0	40%	41%	41%	41%	0%	38%	37%	37%	38%	0%	10%	9%	10%	10%	0%
Leu	[23456]	200	1	19%	19%	19%	19%	0%	39%	39%	39%	39%	0%	3%	2%	3%	3%	0%
Leu	[23456]	200	2	25%	24%	24%	25%	0%	19%	19%	19%	19%	0%	2%	2%	2%	2%	0%
Leu	[23456]	200	3	10%	10%	10%	10%	0%	4%	4%	4%	4%	0%	5%	5%	5%	5%	0%
Leu	[23456]	200	4	5%	5%	5%	5%	0%	0%	0%	0%	0%	0%	15%	14%	15%	14%	0%
Leu	[23456]	200	5	1%	1%	1%	1%	0%	0%	0%	0%	0%	0%	65%	67%	66%	66%	1%
Leu	[23456]	274	0	40%	41%	41%	40%	0%	38%	37%	37%	38%	0%	10%	9%	10%	10%	0%
Leu	[23456]	274	1	19%	19%	19%	19%	0%	39%	39%	39%	39%	0%	2%	2%	2%	2%	0%
Leu	[23456]	274	2	25%	24%	24%	24%	0%	19%	19%	19%	19%	0%	2%	2%	2%	2%	0%
Leu	[23456]	274	3	10%	10%	10%	10%	0%	4%	4%	4%	4%	0%	5%	5%	5%	5%	0%
Leu	[23456]	274	4	5%	5%	5%	5%	0%	0%	0%	0%	0%	0%	15%	14%	15%	15%	0%
Leu	[23456]	274	5	1%	1%	1%	1%	0%	0%	0%	0%	0%	0%	66%	67%	66%	66%	1%
Phe	[23456789]	234	0	26%	26%	26%	26%	0%	33%	33%	33%	33%	0%	6%	5%	6%	6%	0%
Phe	[23456789]	234	1	14%	14%	14%	14%	0%	40%	40%	41%	40%	0%	1%	0%	1%	0%	0%
Phe	[23456789]	234	2	20%	20%	20%	20%	0%	21%	21%	21%	21%	0%	0%	0%	0%	0%	0%
Phe	[23456789]	234	3	16%	16%	16%	16%	0%	5%	5%	5%	5%	0%	0%	0%	0%	0%	0%
Phe	[23456789]	234	4	11%	11%	11%	11%	0%	1%	1%	1%	1%	0%	0%	0%	0%	0%	0%
Phe	[23456789]	234	5	8%	8%	8%	8%	0%	0%	0%	0%	0%	0%	1%	1%	1%	1%	0%
Phe	[23456789]	234	6	4%	4%	4%	4%	0%	0%	0%	0%	0%	0%	3%	3%	3%	3%	0%
Phe	[23456789]	234	7	1%	1%	1%	1%	0%	0%	0%	0%	0%	0%	9%	9%	9%	9%	0%
Phe	[23456789]	234	8	1%	1%	1%	1%	0%	0%	0%	0%	0%	0%	80%	80%	80%	80%	0%
Phe	[12]	302	0	68%	68%	68%	68%	0%	96%	96%	96%	96%	0%	8%	8%	8%	8%	0%
Phe	[12]	302	1	11%	12%	12%	12%	0%	4%	4%	4%	4%	0%	3%	3%	3%	3%	0%
Phe	[12]	302	2	20%	21%	21%	21%	0%	0%	0%	0%	0%	0%	89%	89%	89%	89%	0%
Phe	[123456789	336	0	25%	25%	25%	25%	0%	33%	32%	32%	32%	0%	6%	6%	6%	6%	0%

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Fragments (↓) | Labels (→)				28% U-13C					100% 1-13C					98% U-13C				
AA	frag	MW-frag	n(m+n)	Rep 1	Rep 2	Rep 3	Avg	SD	Rep 1	Rep 2	Rep 3	Avg	SD	Rep 1	Rep 2	Rep 3	Avg	SD
Phe	[12345678	336	1	14%	14%	14%	14%	0%	40%	41%	41%	41%	0%	1%	1%	1%	1%	0%
Phe	[12345678	336	2	14%	14%	14%	14%	0%	21%	22%	22%	22%	0%	0%	0%	0%	0%	0%
Phe	[12345678	336	3	19%	19%	19%	19%	0%	5%	5%	5%	5%	0%	0%	0%	0%	0%	0%
Phe	[12345678	336	4	11%	11%	11%	11%	0%	1%	1%	1%	1%	0%	0%	0%	0%	0%	0%
Phe	[12345678	336	5	8%	8%	8%	8%	0%	0%	0%	0%	0%	0%	1%	0%	0%	0%	0%
Phe	[12345678	336	6	6%	6%	6%	6%	0%	0%	0%	0%	0%	0%	2%	2%	2%	2%	0%
Phe	[12345678	336	7	2%	2%	2%	2%	0%	0%	0%	0%	0%	0%	3%	3%	3%	3%	0%
Phe	[12345678	336	8	1%	1%	1%	1%	0%	0%	0%	0%	0%	0%	10%	10%	10%	10%	0%
Phe	[12345678	336	9	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	78%	78%	78%	78%	0%
Pro	[2345]	258	0	48%	48%	49%	48%	0%	48%	47%	47%	47%	0%	11%	10%	11%	10%	0%
Pro	[2345]	258	1	22%	22%	22%	22%	0%	38%	39%	38%	38%	0%	6%	6%	6%	6%	0%
Pro	[2345]	258	2	22%	22%	22%	22%	0%	13%	13%	13%	13%	0%	12%	12%	12%	12%	0%
Pro	[2345]	258	3	6%	6%	5%	6%	0%	1%	1%	2%	2%	0%	11%	11%	11%	11%	0%
Pro	[2345]	258	4	3%	3%	2%	3%	0%	0%	0%	0%	0%	0%	60%	61%	60%	60%	1%
Ser	[23]	288	0	61%	61%	61%	61%	0%	75%	75%	76%	76%	0%	5%	5%	5%	5%	0%
Ser	[23]	288	1	24%	24%	24%	24%	0%	24%	24%	24%	24%	0%	8%	8%	8%	8%	0%
Ser	[23]	288	2	15%	15%	15%	15%	0%	0%	0%	0%	0%	0%	87%	88%	87%	87%	0%
Ser	[12]	302	0	64%	65%	64%	64%	0%	95%		86%	90%	6%	6%	6%	6%	6%	0%
Ser	[12]	302	1	16%	15%	15%	16%	0%	5%		12%	8%	5%	8%	8%	8%	8%	0%
Ser	[12]	302	2	20%	20%	20%	20%	0%	0%		2%	1%	1%	86%	86%	86%	86%	0%
Ser	[23]	362	0	61%	60%	61%	61%	0%	75%	75%	76%	75%	0%	5%	4%	5%	5%	0%
Ser	[23]	362	1	24%	25%	24%	25%	0%	24%	24%	24%	24%	0%	8%	8%	8%	8%	0%
Ser	[23]	362	2	15%	15%	15%	15%	0%	0%	0%	0%	0%	0%	88%	88%	88%	88%	0%
Ser	[123]	390	0	55%	55%	56%	55%	0%	72%	72%	72%	72%	0%	4%	4%	4%	4%	0%
Ser	[123]	390	1	20%	21%	20%	20%	0%	27%	27%	27%	27%	0%	3%	3%	3%	3%	0%
Ser	[123]	390	2	13%	13%	13%	13%	0%	1%	1%	1%	1%	0%	9%	8%	9%	9%	0%
Ser	[123]	390	3	12%	12%	12%	12%	0%	0%	0%	0%	0%	0%	84%	85%	84%	85%	0%
Thr	[234]	376	0	57%	56%	56%	56%	0%	58%	58%	58%	58%	0%	10%	9%	9%	9%	0%
Thr	[234]	376	1	21%	22%	23%	22%	1%	35%	35%	35%	35%	0%	7%	7%	7%	7%	0%
Thr	[234]	376	2	15%	14%	14%	14%	0%	7%	7%	7%	7%	0%	13%	13%	13%	13%	0%
Thr	[234]	376	3	7%	7%	7%	7%	0%	0%	0%	0%	0%	0%	70%	71%	70%	70%	1%
Thr	[1234]	404	0	48%	50%	49%	49%	1%	51%	51%	51%	51%	0%	8%	8%	8%	8%	0%
Thr	[1234]	404	1	22%	21%	22%	21%	1%	38%	38%	38%	38%	0%	4%	4%	4%	4%	0%
Thr	[1234]	404	2	17%	16%	16%	16%	0%	10%	10%	10%	10%	0%	8%	8%	8%	8%	0%
Thr	[1234]	404	3	9%	10%	10%	10%	0%	1%	1%	1%	1%	0%	14%	14%	14%	14%	0%
Thr	[1234]	404	4	3%	3%	3%	3%	0%	0%	0%	0%	0%	0%	65%	66%	66%	66%	1%
Tyr	[12]	302	0	68%	68%	69%	68%	0%	97%	97%	97%	97%	0%	10%	10%	10%	10%	0%
Tyr	[12]	302	1	11%	11%	11%	11%	0%	3%	3%	3%	3%	0%	3%	3%	3%	3%	0%
Tyr	[12]	302	2	21%	21%	21%	21%	0%	0%	0%	0%	0%	0%	87%	87%	87%	87%	0%
Val	[2345]	186	0	47%	48%	48%	48%	0%	45%	45%	45%	45%	0%	7%	7%	7%	7%	0%

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Fragments (↓) | Labels (→)				28% U-13C					100% 1-13C					98% U-13C				
AA	frag	MW-frag	n(m+n)	Rep 1	Rep 2	Rep 3	Avg	SD	Rep 1	Rep 2	Rep 3	Avg	SD	Rep 1	Rep 2	Rep 3	Avg	SD
Val	[2345]	186	1	11%	11%	11%	11%	0%	40%	40%	41%	40%	0%	1%	1%	1%	1%	0%
Val	[2345]	186	2	30%	30%	30%	30%	0%	12%	12%	12%	12%	0%	4%	4%	4%	4%	0%
Val	[2345]	186	3	6%	6%	6%	6%	0%	2%	2%	2%	2%	0%	9%	9%	9%	9%	0%
Val	[2345]	186	4	5%	5%	5%	5%	0%	0%	0%	0%	0%	0%	79%	80%	79%	79%	0%
Val	[2345]	260	0	48%	48%	48%	48%	0%	46%	46%	45%	46%	0%	7%	7%	7%	7%	0%
Val	[2345]	260	1	12%	12%	12%	12%	0%	41%	41%	42%	41%	0%	1%	1%	1%	1%	0%
Val	[2345]	260	2	30%	30%	30%	30%	0%	12%	12%	12%	12%	0%	4%	4%	4%	4%	0%
Val	[2345]	260	3	4%	4%	4%	4%	0%	1%	1%	1%	1%	0%	8%	8%	8%	8%	0%
Val	[2345]	260	4	5%	5%	5%	5%	0%	0%	0%	0%	0%	0%	79%	80%	79%	80%	0%
Val	[12345]	288	0	45%	46%	46%	46%	0%	45%	45%	44%	45%	0%	7%	7%	7%	7%	0%
Val	[12345]	288	1	12%	13%	13%	13%	0%	41%	41%	41%	41%	0%	1%	1%	1%	1%	0%
Val	[12345]	288	2	19%	19%	19%	19%	0%	13%	13%	13%	13%	0%	2%	2%	2%	2%	0%
Val	[12345]	288	3	16%	15%	16%	16%	0%	1%	1%	1%	1%	0%	4%	4%	4%	4%	0%
Val	[12345]	288	4	3%	3%	3%	3%	0%	0%	0%	0%	0%	0%	8%	8%	8%	8%	0%
Val	[12345]	288	5	5%	4%	4%	4%	0%	0%	0%	0%	0%	0%	78%	79%	78%	78%	1%
Val	[12]	302	0	65%	65%	65%	65%	0%	86%	86%	86%	86%	0%	11%	11%	11%	11%	0%
Val	[12]	302	1	12%	13%	12%	12%	0%	12%	12%	12%	12%	0%	4%	4%	4%	4%	0%
Val	[12]	302	2	23%	22%	23%	23%	0%	2%	2%	2%	2%	0%	85%	85%	85%	85%	0%

Electronic Supplementary Material (ESI) for Molecular BioSystems

Supplementary Tables

Table S2. Isotopomer abundances of intracellular metabolites from poplar cell suspensions grown under light and dark for 7 d.

Fragments (↓) | Labels (→)				98% U-13C, under light							98% U-13C, under dark						
AA	frag	MW-frag	n(m+n)	Rep 1	Rep 2	Rep 3	Avg	SD	13C Enr	SD	Rep 1	Rep 2	Rep 3	Avg	SD	13C Enr	SD
Ala	[23]	232	0	1%	1%	1%	1%	0%	97%	0%	3%	3%	2%	2%	0%	95%	0%
Ala	[23]	232	1	3%	4%	3%	3%	1%	0%	0%	5%	6%	6%	6%	0%	0%	0%
Ala	[23]	232	2	96%	95%	96%	96%	1%	0%	0%	92%	92%	92%	92%	0%	0%	0%
Ala	[123]	260	0	1%	1%	1%	1%	0%	97%	0%	2%	2%	2%	2%	0%	94%	0%
Ala	[123]	260	1	1%	1%	1%	1%	0%	0%	0%	2%	2%	2%	2%	0%	0%	0%
Ala	[123]	260	2	4%	5%	4%	4%	1%	0%	0%	7%	7%	7%	7%	0%	0%	0%
Ala	[123]	260	3	94%	93%	93%	93%	1%	0%	0%	89%	89%	89%	89%	0%	0%	0%
Asp	[12]	302	0	5%	5%	5%	5%	0%	91%	0%	6%	6%	5%	6%	1%	89%	1%
Asp	[12]	302	1	7%	8%	7%	7%	0%	0%	0%	10%	9%	10%	10%	1%	0%	0%
Asp	[12]	302	2	88%	88%	88%	88%	0%	0%	0%	84%	85%	86%	85%	1%	0%	0%
Asp	[234]	316	0	2%	2%	3%	2%	0%	92%	1%	2%	2%	0%	2%	1%	90%	2%
Asp	[234]	316	1	3%	3%	4%	4%	0%	0%	0%	5%	7%	5%	6%	1%	0%	0%
Asp	[234]	316	2	8%	10%	10%	9%	1%	0%	0%	14%	12%	11%	12%	1%	0%	0%
Asp	[234]	316	3	86%	84%	84%	85%	1%	0%	0%	79%	79%	83%	80%	2%	0%	0%
Asp	[234]	390	0	2%	2%	3%	3%	0%	92%	0%	2%	0%	2%	1%	1%	91%	2%
Asp	[234]	390	1	3%	3%	3%	3%	0%	0%	0%	5%	3%	4%	4%	1%	0%	0%
Asp	[234]	390	2	9%	10%	9%	10%	1%	0%	0%	13%	12%	11%	12%	1%	0%	0%
Asp	[234]	390	3	85%	84%	85%	85%	0%	0%	0%	79%	85%	84%	83%	3%	0%	0%
Asp	[1234]	418	0	2%	2%	2%	2%	0%	91%	0%	2%	1%	1%	2%	0%	91%	1%
Asp	[1234]	418	1	1%	1%	2%	1%	0%	0%	0%	2%	2%	1%	2%	0%	0%	0%
Asp	[1234]	418	2	5%	4%	4%	5%	0%	0%	0%	5%	7%	5%	6%	1%	0%	0%
Asp	[1234]	418	3	12%	12%	13%	12%	0%	0%	0%	14%	12%	14%	13%	1%	0%	0%
Asp	[1234]	418	4	80%	81%	79%	80%	1%	0%	0%	77%	77%	78%	78%	0%	0%	0%
Glu	[2345]	272	0	1%	1%	1%	1%	0%	93%	0%	2%	2%	3%	2%	1%	86%	3%
Glu	[2345]	272	1	1%	1%	2%	1%	0%	0%	0%	2%	2%	6%	3%	2%	0%	0%
Glu	[2345]	272	2	5%	5%	5%	5%	0%	0%	0%	9%	10%	11%	10%	1%	0%	0%
Glu	[2345]	272	3	9%	10%	9%	9%	1%	0%	0%	15%	17%	15%	16%	1%	0%	0%
Glu	[2345]	272	4	84%	83%	83%	83%	1%	0%	0%	72%	68%	65%	69%	4%	0%	0%
Glu	[2345]	330	0	1%	1%	1%	1%	0%	93%	0%	3%	3%	0%	2%	2%	86%	2%
Glu	[2345]	330	1	1%	1%	2%	1%	0%	0%	0%	2%	2%	6%	3%	2%	0%	0%
Glu	[2345]	330	2	6%	5%	6%	6%	0%	0%	0%	10%	15%	15%	13%	3%	0%	0%
Glu	[2345]	330	3	9%	10%	9%	9%	0%	0%	0%	13%	13%	15%	13%	1%	0%	0%
Glu	[2345]	330	4	83%	82%	82%	83%	1%	0%	0%	73%	68%	64%	68%	4%	0%	0%
Glu	[12345]	432	0	1%	1%	1%	1%	0%	93%	0%	1%	0%	3%	1%	1%	88%	3%
Glu	[12345]	432	1	1%	1%	1%	1%	0%	0%	0%	2%	1%	2%	2%	1%	0%	0%
Glu	[12345]	432	2	2%	2%	2%	2%	0%	0%	0%	4%	2%	5%	3%	1%	0%	0%
Glu	[12345]	432	3	6%	6%	6%	6%	0%	0%	0%	9%	11%	12%	11%	2%	0%	0%
Glu	[12345]	432	4	11%	12%	11%	11%	0%	0%	0%	15%	17%	15%	16%	1%	0%	0%
Glu	[12345]	432	5	80%	79%	79%	79%	1%	0%	0%	70%	69%	63%	67%	4%	0%	0%
Gly	[2]	218	0	7%	8%	8%	8%	0%	92%	0%	8%	7%	7%	7%	0%	93%	0%

Electronic Supplementary Material (ESI) for Molecular BioSystems

Supplementary Tables

Table S2. Isotopomer abundances of intracellular metabolites from poplar cell suspensions grown under light and dark for 7 d.

Fragments (↓) | Labels (→)				98% U-13C, under light							98% U-13C, under dark						
AA	frag	MW-frag	n(m+n)	Rep 1	Rep 2	Rep 3	Avg	SD	13C Enr	SD	Rep 1	Rep 2	Rep 3	Avg	SD	13C Enr	SD
Gly	[2]	218	1	93%	92%	92%	92%	0%	0%	0%	92%	93%	93%	93%	0%	0%	0%
Gly	[12]	246	0	6%	5%	6%	6%	0%	91%	0%	6%	5%	5%	5%	0%	91%	1%
Gly	[12]	246	1	6%	7%	6%	6%	0%	0%	0%	7%	7%	7%	7%	0%	0%	0%
Gly	[12]	246	2	88%	88%	88%	88%	0%	0%	0%	87%	88%	88%	88%	1%	0%	0%
His	[2345]	196	0	7%	7%	8%	8%	1%	88%	1%	6%	6%	7%	6%	0%	89%	1%
His	[2345]	196	1	1%	1%	1%	1%	0%	0%	0%	1%	1%	1%	1%	0%	0%	0%
His	[2345]	196	2	2%	2%	2%	2%	0%	0%	0%	3%	2%	2%	2%	0%	0%	0%
His	[2345]	196	3	11%	13%	11%	11%	1%	0%	0%	13%	13%	13%	13%	0%	0%	0%
His	[2345]	196	4	79%	77%	78%	78%	1%	0%	0%	77%	78%	77%	77%	1%	0%	0%
His	[23456]	338	0	8%	8%	9%	8%	1%	88%	1%	6%	7%	7%	7%	0%	89%	1%
His	[23456]	338	1	1%	1%	1%	1%	0%	0%	0%	-1%	1%	1%	0%	1%	0%	0%
His	[23456]	338	2	1%	1%	1%	1%	0%	0%	0%	1%	1%	0%	0%	1%	0%	0%
His	[23456]	338	3	2%	3%	3%	3%	0%	0%	0%	2%	4%	5%	4%	2%	0%	0%
His	[23456]	338	4	10%	11%	9%	10%	1%	0%	0%	12%	10%	11%	11%	1%	0%	0%
His	[23456]	338	5	78%	77%	77%	78%	0%	0%	0%	80%	78%	77%	78%	1%	0%	0%
His	[123456]	440	0	7%	7%	8%	8%	1%	88%	1%	6%	7%	6%	6%	1%	90%	0%
His	[123456]	440	1	1%	1%	1%	1%	0%	0%	0%	1%	0%	0%	0%	0%	0%	0%
His	[123456]	440	2	0%	0%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
His	[123456]	440	3	1%	1%	1%	1%	0%	0%	0%	1%	1%	1%	1%	0%	0%	0%
His	[123456]	440	4	2%	2%	2%	2%	0%	0%	0%	2%	1%	2%	2%	1%	0%	0%
His	[123456]	440	5	11%	11%	11%	11%	0%	0%	0%	11%	12%	11%	12%	0%	0%	0%
His	[123456]	440	6	78%	78%	77%	77%	0%	0%	0%	79%	78%	79%	79%	1%	0%	0%
Ile	[23456]	200	0	9%	8%	9%	9%	0%	78%	1%	8%	8%	7%	7%	0%	78%	1%
Ile	[23456]	200	1	2%	2%	2%	2%	0%	0%	0%	1%	1%	1%	1%	0%	0%	0%
Ile	[23456]	200	2	8%	8%	9%	9%	0%	0%	0%	8%	8%	9%	8%	1%	0%	0%
Ile	[23456]	200	3	9%	9%	10%	10%	0%	0%	0%	11%	11%	12%	12%	1%	0%	0%
Ile	[23456]	200	4	14%	15%	14%	14%	1%	0%	0%	17%	18%	19%	18%	1%	0%	0%
Ile	[23456]	200	5	58%	57%	56%	57%	1%	0%	0%	54%	55%	51%	53%	2%	0%	0%
Ile	[23456]	274	0	8%	8%	9%	8%	0%	79%	1%	8%	7%	7%	7%	0%	78%	1%
Ile	[23456]	274	1	2%	2%	2%	2%	0%	0%	0%	1%	1%	2%	1%	0%	0%	0%
Ile	[23456]	274	2	8%	8%	9%	8%	0%	0%	0%	8%	8%	9%	8%	0%	0%	0%
Ile	[23456]	274	3	9%	9%	10%	9%	0%	0%	0%	11%	11%	12%	11%	1%	0%	0%
Ile	[23456]	274	4	14%	15%	14%	14%	1%	0%	0%	17%	17%	19%	18%	1%	0%	0%
Ile	[23456]	274	5	59%	58%	57%	58%	1%	0%	0%	54%	55%	52%	54%	2%	0%	0%
Ile	[12]	302	0	27%	27%	27%	27%	0%	68%	1%	27%	27%	27%	27%	0%	68%	0%
Ile	[12]	302	1	10%	10%	10%	10%	0%	0%	0%	10%	10%	11%	11%	1%	0%	0%
Ile	[12]	302	2	64%	63%	63%	63%	1%	0%	0%	63%	63%	62%	63%	1%	0%	0%
Leu	[23456]	200	0	7%	7%	7%	7%	0%	86%	0%	6%	6%	6%	6%	0%	85%	1%
Leu	[23456]	200	1	2%	2%	2%	2%	0%	0%	0%	1%	1%	1%	1%	0%	0%	0%
Leu	[23456]	200	2	2%	2%	2%	2%	0%	0%	0%	2%	2%	2%	2%	0%	0%	0%

Electronic Supplementary Material (ESI) for Molecular BioSystems

Supplementary Tables

Table S2. Isotopomer abundances of intracellular metabolites from poplar cell suspensions grown under light and dark for 7 d.

Fragments (↓) | Labels (→)				98% U-13C, under light							98% U-13C, under dark						
AA	frag	MW-frag	n(m+n)	Rep 1	Rep 2	Rep 3	Avg	SD	13C Enr	SD	Rep 1	Rep 2	Rep 3	Avg	SD	13C Enr	SD
Leu	[23456]	200	3	4%	5%	4%	4%	0%	0%	0%	5%	5%	6%	5%	0%	0%	0%
Leu	[23456]	200	4	12%	14%	12%	13%	1%	0%	0%	21%	21%	24%	22%	2%	0%	0%
Leu	[23456]	200	5	73%	71%	71%	72%	1%	0%	0%	64%	64%	60%	63%	2%	0%	0%
Leu	[23456]	274	0	7%	7%	7%	7%	0%	86%	0%	6%	6%	6%	6%	0%	85%	1%
Leu	[23456]	274	1	2%	2%	2%	2%	0%	0%	0%	1%	1%	1%	1%	0%	0%	0%
Leu	[23456]	274	2	2%	2%	2%	2%	0%	0%	0%	2%	2%	2%	2%	0%	0%	0%
Leu	[23456]	274	3	4%	4%	4%	4%	0%	0%	0%	5%	5%	5%	5%	0%	0%	0%
Leu	[23456]	274	4	12%	14%	13%	13%	1%	0%	0%	21%	21%	24%	22%	2%	0%	0%
Leu	[23456]	274	5	73%	71%	72%	72%	1%	0%	0%	65%	65%	61%	63%	2%	0%	0%
Lys	[23456]	329	0	7%	13%	10%	10%	3%	77%	0%	9%	4%	14%	9%	5%	77%	3%
Lys	[23456]	329	1	5%	3%	4%	4%	1%	0%	0%	3%	7%	0%	3%	4%	0%	0%
Lys	[23456]	329	2	7%	7%	2%	6%	3%	0%	0%	4%	5%	6%	5%	1%	0%	0%
Lys	[23456]	329	3	11%	13%	14%	13%	1%	0%	0%	18%	9%	12%	13%	5%	0%	0%
Lys	[23456]	329	4	14%	16%	16%	15%	1%	0%	0%	12%	16%	16%	15%	2%	0%	0%
Lys	[23456]	329	5	56%	47%	55%	53%	5%	0%	0%	54%	59%	52%	55%	3%	0%	0%
Lys	[123456]	431	0	7%	13%	11%	10%	3%	78%	2%	6%	6%	7%	6%	0%	76%	2%
Lys	[123456]	431	1	2%	2%	0%	1%	2%	0%	0%	2%	3%	0%	2%	1%	0%	0%
Lys	[123456]	431	2	2%	2%	3%	2%	0%	0%	0%	1%	3%	1%	1%	1%	0%	0%
Lys	[123456]	431	3	5%	6%	5%	6%	1%	0%	0%	4%	4%	7%	5%	2%	0%	0%
Lys	[123456]	431	4	14%	33%	18%	21%	10%	0%	0%	28%	31%	37%	32%	5%	0%	0%
Lys	[123456]	431	5	18%	9%	12%	13%	5%	0%	0%	13%	8%	15%	12%	4%	0%	0%
Lys	[123456]	431	6	52%	34%	51%	46%	10%	0%	0%	47%	45%	33%	42%	7%	0%	0%
Lys	[123456]	488	0	7%	10%	8%	9%	2%	81%	3%	9%	1%	9%	6%	5%	81%	4%
Lys	[123456]	488	1	1%	1%	0%	1%	1%	0%	0%	1%	6%	2%	3%	3%	0%	0%
Lys	[123456]	488	2	4%	-1%	2%	2%	3%	0%	0%	0%	9%	2%	3%	4%	0%	0%
Lys	[123456]	488	3	6%	7%	5%	6%	1%	0%	0%	6%	1%	10%	6%	5%	0%	0%
Lys	[123456]	488	4	11%	11%	7%	9%	3%	0%	0%	11%	5%	8%	8%	3%	0%	0%
Lys	[123456]	488	5	7%	18%	11%	12%	6%	0%	0%	13%	5%	21%	13%	8%	0%	0%
Lys	[123456]	488	6	65%	53%	67%	61%	8%	0%	0%	60%	74%	48%	61%	13%	0%	0%
Met	[2345]	218	0	2%	2%	2%	2%	0%	88%	0%	3%	3%	3%	3%	0%	84%	1%
Met	[2345]	218	1	6%	6%	6%	6%	0%	0%	0%	7%	7%	8%	7%	1%	0%	0%
Met	[2345]	218	2	4%	5%	4%	4%	0%	0%	0%	6%	7%	8%	7%	1%	0%	0%
Met	[2345]	218	3	13%	14%	13%	13%	1%	0%	0%	15%	15%	16%	15%	1%	0%	0%
Met	[2345]	218	4	75%	73%	75%	74%	1%	0%	0%	69%	68%	66%	68%	2%	0%	0%
Met	[2345]	292	0	1%	2%	2%	2%	0%	89%	0%	1%	2%	1%	2%	0%	87%	1%
Met	[2345]	292	1	5%	5%	5%	5%	0%	0%	0%	6%	5%	7%	6%	1%	0%	0%
Met	[2345]	292	2	4%	4%	4%	4%	0%	0%	0%	6%	6%	8%	6%	1%	0%	0%
Met	[2345]	292	3	14%	15%	14%	14%	1%	0%	0%	15%	15%	16%	15%	1%	0%	0%
Met	[2345]	292	4	75%	75%	75%	75%	0%	0%	0%	73%	73%	68%	71%	3%	0%	0%
Met	[12345]	320	0	1%	2%	1%	1%	1%	89%	0%	1%	2%	2%	1%	0%	88%	2%

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Supplementary Tables

Table S2. Isotopomer abundances of intracellular metabolites from poplar cell suspensions grown under light and dark for 7 d.

Fragments (↓) | Labels (→)				98% U-13C, under light							98% U-13C, under dark						
AA	frag	MW-frag	n(m+n)	Rep 1	Rep 2	Rep 3	Avg	SD	13C Enr	SD	Rep 1	Rep 2	Rep 3	Avg	SD	13C Enr	SD
Met	[12345]	320	1	5%	4%	5%	4%	0%	0%	0%	4%	2%	5%	4%	1%	0%	0%
Met	[12345]	320	2	2%	2%	3%	2%	0%	0%	0%	2%	3%	5%	3%	2%	0%	0%
Met	[12345]	320	3	4%	5%	4%	5%	0%	0%	0%	5%	7%	8%	7%	2%	0%	0%
Met	[12345]	320	4	14%	16%	14%	14%	1%	0%	0%	17%	17%	16%	17%	0%	0%	0%
Met	[12345]	320	5	74%	72%	74%	73%	1%	0%	0%	72%	70%	64%	68%	4%	0%	0%
Phe	[23456789]	234	0	3%	4%	4%	4%	0%	94%	0%	2%	2%	2%	2%	0%	95%	0%
Phe	[23456789]	234	1	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Phe	[23456789]	234	2	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Phe	[23456789]	234	3	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Phe	[23456789]	234	4	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Phe	[23456789]	234	5	1%	1%	1%	1%	0%	0%	0%	1%	1%	1%	1%	0%	0%	0%
Phe	[23456789]	234	6	3%	3%	3%	3%	0%	0%	0%	4%	4%	4%	4%	0%	0%	0%
Phe	[23456789]	234	7	8%	9%	8%	8%	1%	0%	0%	10%	10%	10%	10%	0%	0%	0%
Phe	[23456789]	234	8	84%	82%	84%	83%	1%	0%	0%	82%	83%	82%	82%	0%	0%	0%
Phe	[12]	302	0	5%	5%	6%	5%	0%	93%	0%	4%	4%	4%	4%	0%	94%	0%
Phe	[12]	302	1	3%	3%	3%	3%	0%	0%	0%	3%	3%	3%	3%	0%	0%	0%
Phe	[12]	302	2	92%	91%	91%	92%	0%	0%	0%	93%	93%	92%	93%	0%	0%	0%
Phe	[123456789	336	0	4%	4%	4%	4%	0%	93%	0%	2%	2%	2%	2%	0%	95%	0%
Phe	[123456789	336	1	0%	0%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Phe	[123456789	336	2	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Phe	[123456789	336	3	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Phe	[123456789	336	4	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Phe	[123456789	336	5	0%	0%	0%	0%	0%	0%	0%	1%	0%	0%	0%	0%	0%	0%
Phe	[123456789	336	6	2%	2%	2%	2%	0%	0%	0%	2%	2%	2%	2%	0%	0%	0%
Phe	[123456789	336	7	2%	2%	2%	2%	0%	0%	0%	3%	3%	3%	3%	0%	0%	0%
Phe	[123456789	336	8	9%	10%	9%	9%	1%	0%	0%	10%	10%	11%	10%	0%	0%	0%
Phe	[123456789	336	9	82%	81%	82%	82%	1%	0%	0%	81%	82%	81%	81%	0%	0%	0%
Pro	[2345]	184	0	8%	8%	9%	8%	0%	79%	0%	8%	7%	8%	8%	0%	76%	2%
Pro	[2345]	184	1	5%	5%	6%	5%	0%	0%	0%	6%	6%	8%	7%	1%	0%	0%
Pro	[2345]	184	2	11%	11%	12%	12%	0%	0%	0%	14%	14%	16%	15%	1%	0%	0%
Pro	[2345]	184	3	11%	11%	10%	11%	0%	0%	0%	14%	14%	15%	15%	0%	0%	0%
Pro	[2345]	184	4	64%	64%	63%	64%	1%	0%	0%	58%	58%	53%	56%	3%	0%	0%
Pro	[2345]	258	0	5%	4%	5%	4%	0%	87%	0%	3%	4%	4%	4%	0%	84%	1%
Pro	[2345]	258	1	3%	3%	3%	3%	0%	0%	0%	4%	4%	5%	4%	1%	0%	0%
Pro	[2345]	258	2	8%	8%	8%	8%	0%	0%	0%	11%	11%	12%	11%	1%	0%	0%
Pro	[2345]	258	3	10%	10%	9%	10%	1%	0%	0%	13%	14%	14%	14%	0%	0%	0%
Pro	[2345]	258	4	74%	75%	75%	74%	0%	0%	0%	68%	68%	66%	67%	1%	0%	0%
Ser	[23]	288	0	2%	2%	2%	2%	0%	94%	0%	2%	2%	2%	2%	0%	95%	0%
Ser	[23]	288	1	7%	8%	7%	8%	0%	0%	0%	6%	7%	6%	6%	0%	0%	0%
Ser	[23]	288	2	91%	90%	91%	91%	0%	0%	0%	92%	91%	92%	92%	1%	0%	0%

Electronic Supplementary Material (ESI) for Molecular BioSystems

Supplementary Tables

Table S2. Isotopomer abundances of intracellular metabolites from poplar cell suspensions grown under light and dark for 7 d.

Fragments (↓) | Labels (→)				98% U-13C, under light							98% U-13C, under dark						
AA	frag	MW-frag	n(m+n)	Rep 1	Rep 2	Rep 3	Avg	SD	13C Enr	SD	Rep 1	Rep 2	Rep 3	Avg	SD	13C Enr	SD
Ser	[12]	302	0	3%	4%	4%	4%	0%	93%	1%	4%	3%	4%	4%	0%	92%	0%
Ser	[12]	302	1	6%	9%	7%	8%	2%	0%	0%	9%	10%	9%	9%	0%	0%	0%
Ser	[12]	302	2	90%	87%	89%	89%	2%	0%	0%	87%	87%	87%	87%	0%	0%	0%
Ser	[23]	362	0	2%	2%	2%	2%	0%	95%	0%	2%	2%	2%	2%	0%	95%	0%
Ser	[23]	362	1	7%	8%	7%	7%	0%	0%	0%	6%	6%	6%	6%	0%	0%	0%
Ser	[23]	362	2	92%	91%	91%	91%	0%	0%	0%	92%	92%	92%	92%	0%	0%	0%
Ser	[123]	390	0	1%	1%	2%	2%	0%	94%	0%	2%	2%	2%	2%	0%	94%	0%
Ser	[123]	390	1	2%	2%	2%	2%	0%	0%	0%	2%	2%	2%	2%	0%	0%	0%
Ser	[123]	390	2	7%	9%	8%	8%	1%	0%	0%	8%	7%	7%	7%	1%	0%	0%
Ser	[123]	390	3	89%	88%	88%	88%	1%	0%	0%	88%	89%	90%	89%	1%	0%	0%
Thr	[234]	376	0	7%	7%	8%	7%	0%	84%	1%	7%	8%	7%	7%	1%	83%	3%
Thr	[234]	376	1	7%	7%	7%	7%	0%	0%	0%	9%	-1%	10%	6%	6%	0%	0%
Thr	[234]	376	2	12%	12%	12%	12%	0%	0%	0%	16%	17%	18%	17%	1%	0%	0%
Thr	[234]	376	3	74%	74%	72%	73%	1%	0%	0%	68%	75%	65%	69%	5%	0%	0%
Thr	[1234]	404	0	7%	6%	7%	7%	0%	83%	1%	6%	7%	7%	6%	0%	81%	2%
Thr	[1234]	404	1	3%	3%	3%	3%	0%	0%	0%	5%	4%	6%	5%	1%	0%	0%
Thr	[1234]	404	2	7%	7%	8%	7%	0%	0%	0%	10%	9%	12%	10%	1%	0%	0%
Thr	[1234]	404	3	13%	14%	14%	14%	0%	0%	0%	15%	17%	16%	16%	1%	0%	0%
Thr	[1234]	404	4	69%	69%	68%	69%	1%	0%	0%	65%	63%	59%	62%	3%	0%	0%
Tyr	[12]	302	0	8%	8%	8%	8%	0%	91%	0%	7%	7%	7%	7%	0%	91%	0%
Tyr	[12]	302	1	3%	3%	2%	3%	1%	0%	0%	4%	3%	3%	4%	0%	0%	0%
Tyr	[12]	302	2	90%	89%	90%	90%	0%	0%	0%	89%	89%	89%	89%	0%	0%	0%
Tyr	[23456789]	364	0	6%	6%		6%	0%	90%	0%	5%	5%	5%	5%	0%	92%	1%
Tyr	[23456789]	364	1	1%	1%		1%	0%	0%	0%	1%	0%	1%	1%	0%	0%	0%
Tyr	[23456789]	364	2	0%	0%		0%	0%	0%	0%	0%	1%	0%	0%	1%	0%	0%
Tyr	[23456789]	364	3	0%	0%		0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Tyr	[23456789]	364	4	0%	0%		0%	0%	0%	0%	0%	1%	0%	0%	0%	0%	0%
Tyr	[23456789]	364	5	1%	1%		1%	1%	0%	0%	1%	1%	1%	1%	0%	0%	0%
Tyr	[23456789]	364	6	4%	4%		4%	0%	0%	0%	5%	2%	3%	3%	2%	0%	0%
Tyr	[23456789]	364	7	11%	9%		10%	1%	0%	0%	10%	12%	8%	10%	2%	0%	0%
Tyr	[23456789]	364	8	78%	78%		78%	0%	0%	0%	78%	78%	82%	79%	2%	0%	0%
Tyr	[12345678	466	0	5%	5%		5%	0%	92%	0%	6%		4%	5%	1%	91%	1%
Tyr	[12345678	466	1	1%	1%		1%	0%	0%	0%	1%		1%	1%	1%	0%	0%
Tyr	[12345678	466	2	-1%	0%		0%	1%	0%	0%	0%		0%	0%	0%	0%	0%
Tyr	[12345678	466	3	1%	0%		0%	0%	0%	0%	0%		0%	0%	0%	0%	0%
Tyr	[12345678	466	4	0%	0%		0%	0%	0%	0%	0%		0%	0%	0%	0%	0%
Tyr	[12345678	466	5	1%	0%		0%	0%	0%	0%	0%		0%	0%	0%	0%	0%
Tyr	[12345678	466	6	0%	1%		1%	1%	0%	0%	2%		2%	2%	0%	0%	0%
Tyr	[12345678	466	7	3%	3%		3%	0%	0%	0%	3%		3%	3%	0%	0%	0%
Tyr	[12345678	466	8	9%	9%		9%	0%	0%	0%	11%		9%	10%	1%	0%	0%

Electronic Supplementary Material (ESI) for Molecular BioSystems

Supplementary Tables

Table S2. Isotopomer abundances of intracellular metabolites from poplar cell suspensions grown under light and dark for 7 d.

Fragments (↓) | Labels (→)				98% U-13C, under light							98% U-13C, under dark						
AA	frag	MW-frag	n(m+n)	Rep 1	Rep 2	Rep 3	Avg	SD	13C Enr	SD	Rep 1	Rep 2	Rep 3	Avg	SD	13C Enr	SD
Tyr	[123456789	466	9	81%	80%		80%	1%	0%	0%	78%		79%	78%	1%	0%	0%
Val	[2345]	186	0	4%	4%	5%	5%	0%	91%	0%	5%	5%	5%	5%	0%	90%	0%
Val	[2345]	186	1	1%	1%	1%	1%	0%	0%	0%	1%	1%	1%	1%	0%	0%	0%
Val	[2345]	186	2	3%	3%	4%	3%	0%	0%	0%	4%	4%	4%	4%	0%	0%	0%
Val	[2345]	186	3	7%	10%	7%	8%	1%	0%	0%	10%	10%	11%	11%	1%	0%	0%
Val	[2345]	186	4	84%	82%	83%	83%	1%	0%	0%	80%	80%	79%	80%	1%	0%	0%
Val	[2345]	260	0	4%	5%	5%	5%	0%	91%	0%	5%	5%	5%	5%	0%	90%	0%
Val	[2345]	260	1	1%	1%	1%	1%	0%	0%	0%	1%	1%	1%	1%	0%	0%	0%
Val	[2345]	260	2	3%	3%	4%	3%	0%	0%	0%	4%	4%	4%	4%	0%	0%	0%
Val	[2345]	260	3	6%	7%	7%	7%	1%	0%	0%	8%	8%	8%	8%	0%	0%	0%
Val	[2345]	260	4	85%	84%	84%	84%	1%	0%	0%	83%	82%	82%	82%	0%	0%	0%
Val	[12345]	288	0	5%	4%	5%	5%	0%	91%	0%	5%	5%	5%	5%	0%	90%	0%
Val	[12345]	288	1	1%	1%	1%	1%	0%	0%	0%	0%	0%	1%	0%	0%	0%	0%
Val	[12345]	288	2	1%	2%	2%	2%	0%	0%	0%	2%	2%	2%	2%	0%	0%	0%
Val	[12345]	288	3	3%	3%	3%	3%	0%	0%	0%	4%	3%	4%	4%	0%	0%	0%
Val	[12345]	288	4	6%	8%	7%	7%	1%	0%	0%	8%	8%	9%	8%	0%	0%	0%
Val	[12345]	288	5	84%	82%	83%	83%	1%	0%	0%	81%	81%	80%	81%	1%	0%	0%
Val	[12]	302	0	7%	7%	8%	8%	0%	91%	0%	9%	9%	9%	9%	0%	90%	1%
Val	[12]	302	1	3%	4%	3%	4%	0%	0%	0%	0%	3%	4%	2%	3%	0%	0%
Val	[12]	302	2	89%	89%	89%	89%	1%	0%	0%	91%	88%	87%	89%	2%	0%	0%

Electronic Supplementary Material (ESI) for Molecular BioSystems

Supplementary Tables

Table S3. Metabolic fluxes estimated through the four metabolic models.

Iso_corr(U)			Gluc_dilu			Iso_corr(V)			AA_in		
Reaction	**Avg**	**SD**	**Reaction**	**Avg**	**SD**				**Reaction**	**Avg**	**SD**
glci	0.5604	0.0080	glci	0.5508	0.0017	glci	0.5713	0.0123	glci	0.5698	0.0105
CO2in	0.1594	0.0046	CO2in	0.1283	0.0058	CO2in	0.9024	0.0687	CO2in	0.1862	0.1570
CO2out	1.9886	0.0697	CO2out	2.0405	0.0407	CO2out	3.0591	0.1274	CO2out	2.4669	0.1774
									CO2exf	-0.1429	0.1573
									CO2exb	0.7763	0.2601
						Alai	0.0002	0.0001	Alai	0.0018	0.0017
						aspi	0.0011	0.0001	aspi	0.0016	0.0004
						glui	0.0012	0.0001	glui	0.0011	0.0012
						Glyi	0.0001	0.0001	Glyi	0.0003	0.0003
						hisi	0.0001	0.0000	hisi	0.0001	0.0000
						Ile	0.0010	0.0001	Ile	0.0008	0.0001
						Meti	0.0001	0.0001	Meti	0.0001	0.0001
						seri	0.0007	0.0001	seri	0.0007	0.0003
						thri	0.0001	0.0001	thri	0.0003	0.0001
						Vali	0.0021	0.0002	Vali	0.0016	0.0004
						leu	0.0025	0.0001	leu	0.0019	0.0001
									pyrpi	0.0008	0.0002
									OAAmi	0.0025	0.0015
									pyr	0.0009	0.0004
									suci	0.0078	0.0013
									starchi	0.0044	0.0006
									T3Ppi	0.0024	0.0012
									E4Ppi	0.0014	0.0008
									ACApi	0.0094	0.0011
			glcina	0.0237	0.0002				ACAin	0.0083	0.0031
			glcc2	0.0237	0.0002				ACAtf	0.0083	0.0031
pgif	0.1709	0.0508	pgif	0.1625	0.0457	pgif	0.3924	0.0846	pgif	0.3577	0.1008
pgib	0.9334	0.0514	pgib	0.8852	0.0778	pgib	0.4740	0.2885	pgib	0.3712	0.3095
g6pdh	0.2430	0.0945	g6pdh	0.3683	0.0487	g6pdh	0.1092	0.0657	g6pdh	0.1651	0.0709
tktAf	0.0674	0.0217	tktAf	0.1051	0.0220	tktAf	-0.0459	0.0356	tktAf	-0.0130	0.0647
tktAb	0.5347	0.2868	tktAb	0.2864	0.2411	tktAb	0.0880	0.1443	tktAb	0.3276	0.3125
talf	0.0674	0.0217	talf	0.1051	0.0220	talf	-0.0459	0.0356	talf	-0.0130	0.0647
talb	0.5207	0.3118	talb	0.2933	0.2745	talb	0.6646	0.3356	talb	0.7689	0.2946
tktBf	0.0674	0.0217	tktBf	0.1051	0.0220	tktBf	-0.0532	0.0341	tktBf	-0.0184	0.0647
tktBb	0.3079	0.2150	tktBb	0.2863	0.2506	tktBb	0.9373	0.0405	tktBb	0.7768	0.2193
pfk	0.2865	0.0480	pfk	0.3531	0.0607	pfk	0.2667	0.0481	pfk	0.3071	0.0659
f16bp	0.9248	0.0681	f16bp	0.6208	0.2342	f16bp	0.7474	0.0849	f16bp	0.5756	0.1958
pyrf	0.6546	0.0373	pyrf	0.0000	0.0000	pyrf	0.8826	0.2968	pyrf	0.8414	0.2060
g6pt	0.1464	0.1138	g6pt	0.0436	0.0700	g6pt	0.0697	0.0901	g6pt	0.0470	0.0591
g6ptb	0.5937	0.2248	g6ptb	0.6100	0.3604	g6ptb	0.4748	0.2185	g6ptb	0.2965	0.2715
pgifp	-0.5388	0.1164	pgifp	-0.0267	0.0694	pgifp	-0.7036	0.1867	pgifp	-0.4002	0.2359
pgibp	0.3406	0.2888	pgibp	0.5990	0.3288	pgibp	0.8579	0.1119	pgibp	0.8545	0.2269
g6pdhp	0.6635	0.0967	g6pdhp	0.0473	0.0070	g6pdhp	0.7531	0.1938	g6pdhp	0.4301	0.2293
tktAfp	0.2367	0.0437	tktAfp	0.0355	0.0321	tktAfp	0.3354	0.0757	tktAfp	0.2128	0.1120
tktAbp	0.1546	0.1931	tktAbp	0.3758	0.2754	tktAbp	0.9889	0.0203	tktAbp	0.9950	0.0120
talfp	0.2367	0.0437	talfp	0.0355	0.0321	talfp	0.3354	0.0757	talfp	0.2128	0.1120
talbp	0.2584	0.2911	talbp	0.5037	0.3291	talbp	0.9687	0.0331	talbp	0.9847	0.0264
tktBfp	0.2297	0.0434	tktBfp	0.0279	0.0313	tktBfp	0.3354	0.0757	tktBfp	0.2128	0.1120
tktBbp	0.0960	0.1268	tktBbp	0.4942	0.3271	tktBbp	0.7960	0.2242	tktBbp	0.8536	0.2291
pfkp	-0.0724	0.0555	pfkp	0.0367	0.0593	pfkp	0.0254	0.0554	pfkp	0.0254	0.0554
f16bpp	0.7685	0.1209	f16bpp	0.5604	0.3289	f16bpp	0.1769	0.2562	f16bpp	0.3931	0.2452
pepfp	0.0749	0.0301	pepfp	0.9111	0.0585	pepfp	0.2422	0.2450	pepfp	0.1374	0.1409

Electronic Supplementary Material (ESI) for Molecular BioSystems

Supplementary Tables

Table S3. Metabolic fluxes estimated through the four metabolic models.

Iso_corr(U)			Gluc_dilu			Iso_corr(V)			AA_in		
Reaction	**Avg**	**SD**	**Reaction**	**Avg**	**SD**				**Reaction**	**Avg**	**SD**
pdhp	0.2296	0.0037	pdhp	0.2312	0.0026	pdhp	0.2266	0.0030	pdhp	0.2164	0.0033
t3pt	-0.0176	0.1039	t3pt	-0.8401	0.1548	t3pt	0.0168	0.2477	t3pt	0.1159	0.1636
t3pb	0.2802	0.2850	t3pb	0.0486	0.1576	t3pb	0.1761	0.2525	t3pb	0.0944	0.1899
P5Ptf	0.0410	0.1280	P5Ptf	0.0531	0.0973	P5Ptf	0.2542	0.0882	P5Ptf	0.2096	0.1437
P5Ptr	0.6841	0.3162	P5Ptr	0.5951	0.3308	P5Ptr	0.0422	0.0645	P5Ptr	0.0481	0.1297
pyrtpf	0.2223	0.0314	pyrtpf	-0.6121	0.0586	pyrtpf	0.0414	0.2440	pyrtpf	0.1601	0.1471
pyrtpr	0.4049	0.2644	pyrtpr	0.4663	0.3775	pyrtpr	0.8668	0.2177	pyrtpr	0.7409	0.3746
pdh	0.3211	0.0385	pdh	0.5022	0.0204	pdh	0.3685	0.0436	pdh	0.4844	0.0616
citdh	0.3211	0.0385	citdh	0.5022	0.0204	citdh	0.3685	0.0436	citdh	0.4927	0.0627
akgdh	0.2749	0.0394	akgdh	0.4553	0.0216	akgdh	0.3389	0.0427	akgdh	0.4623	0.0626
sdhf	0.2749	0.0394	sdhf	0.4553	0.0216	sdhf	0.3389	0.0427	sdhf	0.4735	0.0586
sdhr	0.9638	0.0257	sdhr	0.9366	0.0442	sdhr	0.9859	0.0154	sdhr	0.9596	0.0378
sdhs	0.6807	0.2441	sdhs	0.6774	0.2549	sdhs	0.6570	0.3330	sdhs	0.3905	0.3322
mdhf	0.3283	0.0444	mdhf	0.4920	0.0465	mdhf	0.6244	0.2189	mdhf	0.4902	0.1463
mdhr	0.9627	0.0227	mdhr	0.9493	0.0474	mdhr	0.9337	0.0887	mdhr	0.9339	0.1436
mef	-0.0534	0.0357	mef	-0.0367	0.0423	mef	-0.2856	0.1947	mef	-0.0167	0.1329
mer	0.2691	0.2769	mer	0.6386	0.2282	mer	0.2663	0.1885	mer	0.3278	0.2335
pyrc	0.0452	0.0268	pyrc	0.0602	0.0246	pyrc	0.1722	0.2276	pyrc	0.1676	0.1103
pepck	0.0340	0.0474	pepck	0.0310	0.0525	pepck	0.4012	0.1340	pepck	0.1410	0.0875
pepc	0.9710	0.0163	pepc	0.9218	0.0353	pepc	0.1748	0.2070	pepc	0.1850	0.2102
						mgdhf	0.0296	0.0023	mgdhf	0.0303	0.0026
									mgdhr	0.7068	0.3379
Serf	0.0115	0.0004	Serf	0.0116	0.0004	Serf	0.0104	0.0007	Serf	0.0104	0.0007
Serb	0.9704	0.0185	Serb	0.9277	0.0591				Serb	0.5454	0.2438
Glyf	0.0076	0.0004	Glyf	0.0077	0.0004	Glyf	0.0074	0.0005	Glyf	0.0072	0.0006
Glyr	0.9805	0.0123	Glyr	0.9456	0.0558	Glyr	0.6071	0.0221	Glyr	0.7329	0.0979
						alaf	0.0124	0.0008	alaf	0.0109	0.0017
									alar	0.8792	0.1874
						aspf	0.0148	0.0004	aspf	0.0144	0.0005
									aspr	0.3232	0.1765
						hisf	0.0011	0.0003	hisf	0.0012	0.0003
						ilef	0.0064	0.0001	ilef	0.0066	0.0001
						metf	0.0009	0.0001	metf	0.0009	0.0001
						thrf	0.0091	0.0001	thrf	0.0090	0.0001
						valf	0.0239	0.0002	valf	0.0363	0.0090
									valcat	0.0112	0.0094
						leu3f	0.0181	0.0001	leu3f	0.0187	0.0002
T3Ppo	0.0162	0.0042	T3Ppo	0.0188	0.0028						
T3Po	0.0021	0.0001	T3Po	0.0021	0.0001						
Sero	0.0039	0.0001	Sero	0.0039	0.0001	Sero	0.0040	0.0001	Sero	0.0039	0.0001
Glyo	0.0076	0.0004	Glyo	0.0077	0.0004	Glyo	0.0075	0.0005	Glyo	0.0075	0.0004
E4Ppo	0.0069	0.0025	E4Ppo	0.0076	0.0023	E4Po	0.0073	0.0025	E4Po	0.0067	0.0021
Pyro	0.0126	0.0007	pyro	0.0129	0.0006	pyro	0.0027	0.0002	pyro	0.0026	0.0002
pyrpo	0.0676	0.0005	pyrpo	0.0678	0.0004	pyrpo	0.0026	0.0001	pyrpo	0.0026	0.0001
ACApo	0.2296	0.0037	ACApo	0.2312	0.0026						
OAAmo	0.0185	0.0013	OAAmo	0.0191	0.0015	OAAmo	0.0112	0.0011	OAAmo	0.0113	0.0009
Gluco	0.0461	0.0037	2OGmo	0.0469	0.0036						
G6Ppout	0.0217	0.0021	G6Ppo	0.0230	0.0020						
P5Ppout	0.0014	0.0004	P5Ppo	0.0015	0.0004						
F6Po	0.0191	0.0009	F6Po	0.0195	0.0007						
CHOo	0.0076	0.0004	CHOo	0.0077	0.0004	CHOo	0.0054	0.0005	CHOo	0.0050	0.0007
						Alao	0.0127	0.0008	Alao	0.0127	0.0006

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Table S3. Metabolic fluxes estimated through the four metabolic models.

Iso_corr(U)			Gluc_dilu			Iso_corr(V)			AA_in		
Reaction	Avg	SD	Reaction	Avg	SD				Reaction	Avg	SD
						Aspo	0.0068	0.0004	Aspo	0.0070	0.0003
						Gluo	0.0308	0.0024	Gluo	0.0314	0.0022
						Hiso	0.0012	0.0003	Hiso	0.0013	0.0003
						Ileo	0.0074	0.0000	Ileo	0.0075	0.0001
						Meto	0.0010	0.0001	Meto	0.0010	0.0001
						Thro	0.0027	0.0000	Thro	0.0026	0.0001
						Valo	0.0080	0.0001	Valo	0.0080	0.0001
						Leuo	0.0206	0.0001	Leuo	0.0206	0.0001
						suco	0.0266	0.0013	suco	0.0270	0.0014
						starcho	0.0203	0.0022	starcho	0.0215	0.0019
						lipid	0.2086	0.0031	lipid	0.2071	0.0030

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Table S4. Metabolic network model incorporating uniform isotopomer correction (Iso_corr[U]).

	Reaction	Net flux	Flux SD	Reversibility
glci	→ Glc	0.5604	0.0080	
CO2in	→ CO_2	0.1594	0.0046	
CO2out	CO_2 →	1.9886	0.0697	
pgif	G6P (123456) → F6P (123456)	0.1709	0.0508	0.9334
g6pdh	G6P (123456) → P5P (23456)	0.2430	0.0945	
tktAf	P5P (12345) + P5P (67890) → S7P (1267890) + T3P (345)	0.0674	0.0217	0.5347
talf	S7P (1234567) + T3P (890) → F6P (123890) + E4P (4567)	0.0674	0.0217	0.5207
tktBf	P5P (12345) + E4P (6789) → F6P (126789) + T3P (345)	0.0674	0.0217	0.3079
pfk	F6P (123456) → T3P (321) + T3P (456)	0.2865	0.0480	0.9248
pyrf	T3P (123) → Pyr (123)	0.6546	0.0373	
g6pt	G6P (123456) → $G6P_p$ (123456)	0.1464	0.1138	0.5937
pgifp	$G6P_p$ (123456) → $F6P_p$ (123456)	-0.5388	0.1164	0.3406
g6pdhp	$G6P_p$ (123456) → $P5P_p$ (23456) + CO_2 (1)	0.6635	0.0967	
tktAfp	$P5P_p$ (12345) + $P5P_p$ (67890) → $S7P_p$ (1267890) + $T3P_p$ (345)	0.2367	0.0437	0.1546
talfp	$S7P_p$ (1234567) + $T3P_p$ (890) → $F6P_p$ (123890) + $E4P_p$ (4567)	0.2367	0.0437	0.2584
tktBfp	$P5P_p$ (12345) + $E4P_p$ (6789) → $F6P_p$ (126789) + $T3P_p$ (345)	0.2297	0.0434	0.0960
pfkp	$F6P_p$ (123456) → $T3P_p$ (321) + $T3P_p$ (456)	-0.0724	0.0555	0.7685
pepfp	$T3P_p$ (123) → Pyr_p (123)	0.0749	0.0301	
pdhp	Pyr_p (123) → Aca_p (23)	0.2296	0.0037	
t3pt	$T3P_p$ (123) → T3P (123)	-0.0176	0.1039	0.2802
P5Ptf	P5P (12345) → $P5P_p$ (12345)	0.0410	0.1280	0.6841
pyrtpf	Pyr (123) → Pyr_p (123)	0.2223	0.0314	0.4039
pdh	Pyr (123) → Aca_m (23)	0.3211	0.0385	
citdh	Aca_m (12) + Oaa_m (3456) → Akg_m (65421) + CO_2 (3)	0.3211	0.0385	
akgdh	Akg_m (12345) → Suc_m (2345) + CO_2 (1)	0.2749	0.0394	
sdhf	Suc_m (1234) → Mal_m (1234)	0.2749	0.0394	0.9638
sdhs	Suc_m (1234) → Mal_m (4321)	0.6807	0.2441	
mdhf	Mal_m (1234) → Oaa_m (1234)	0.3283	0.0444	0.9627
mef	Mal_m (1234) → Pyr (123) + CO_2 (4)	-0.0534	0.0357	0.2691
pyrc	Pyr (123) + CO_2 (4) → Oaa_m (1234)	0.0452	0.0268	
pepck	Oaa_m (1234) → T3P (123) + CO_2 (4)	0.0340	0.0474	0.9710
Serf	$T3P_p$ (123) → Ser (123)	0.0115	0.0004	0.9704
Glyf	Ser (123) → Gly (12) + CHO (3)	0.0076	0.0004	0.9805
T3Ppo	$T3P_p$ →	0.0162	0.0042	
T3Po	T3P →	0.0021	0.0001	
Sero	Ser →	0.0039	0.0001	
Glyo	Gly →	0.0076	0.0004	
E4Ppo	$E4P_p$ →	0.0069	0.0025	
Pyro	Pyr →	0.0126	0.0007	
pyrpo	Pyr_p →	0.0676	0.0005	
ACApo	Aca_p →	0.2296	0.0037	
OAAmo	Oaa_m →	0.0185	0.0013	
Gluco	Akg →	0.0461	0.0037	
G6Ppout	$G6P_p$ →	0.0217	0.0021	
P5Ppout	$P5P_p$ →	0.0014	0.0004	
F6Po	F6P →	0.0191	0.0009	
CHOout	CHO →	0.0076	0.0004	

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Table S5. Metabolic network model incorporating glucose dilution (Gluc_dilu).

	Reaction	Net flux	Flux SD	Reversibility
glci	→ G6P	0.5508	0.0017	
CO2in	→ CO_2	0.1283	0.0058	
CO2out	CO_2 →	2.0405	0.0407	
glcina	→ G6Pn	0.0237	0.0002	
glcc2	G6Pn → G6P	0.0237	0.0002	
pgif	G6P (123456) → F6P (123456)	0.1625	0.0457	0.8852
g6pdh	G6P (123456) → P5P (23456)	0.3683	0.0487	
tktAf	P5P (12345) + P5P (67890) → S7P (1267890) + T3P (345)	0.1051	0.0220	0.2864
talf	S7P (1234567) + T3P (890) → F6P (123890) + E4P (4567)	0.1051	0.0220	0.2933
tktBf	P5P (12345) + E4P (6789) → F6P (126789) + T3P (345)	0.1051	0.0220	0.2863
pfk	F6P (123456) → T3P (321) + T3P (456)	0.3531	0.0607	0.6208
pyrf	T3P (123) → Pyr (123)	0.0000	0.0000	
g6pt	G6P (123456) → $G6P_p$ (123456)	0.0436	0.0700	0.6100
pgifp	$G6P_p$ (123456) → $F6P_p$ (123456)	-0.0267	0.0694	0.5990
g6pdhp	$G6P_p$ (123456) → $P5P_p$ (23456) + CO_2 (1)	0.0473	0.0070	
tktAfp	$P5P_p$ (12345) + $P5P_p$ (67890) → $S7P_p$ (1267890) + $T3P_p$ (345)	0.0355	0.0321	0.3758
talfp	$S7P_p$ (1234567) + $T3P_p$ (890) → $F6P_p$ (123890) + $E4P_p$ (4567)	0.0355	0.0321	0.5037
tktBfp	$P5P_p$ (12345) + $E4P_p$ (6789) → $F6P_p$ (126789) + $T3P_p$ (345)	0.0279	0.0313	0.4942
pfkp	$F6P_p$ (123456) → $T3P_p$ (321) + $T3P_p$ (456)	0.0367	0.0593	0.5604
pepfp	$T3P_p$ (123) → Pyr_p (123)	0.9111	0.0585	
pdhp	Pyr_p (123) → Aca_p (23)	0.2312	0.0026	
t3pt	$T3P_p$ (123) → T3P (123)	-0.8401	0.1548	0.0486
P5Ptf	P5P (12345) → $P5P_p$ (12345)	0.0531	0.0973	0.5951
pyrtpf	Pyr (123) → Pyr_p (123)	-0.6121	0.0586	0.4663
pdh	Pyr (123) → Aca_m (23)	0.5022	0.0204	
citdh	Aca_m (12) + Oaa_m (3456) → Akg_m (65421) + CO_2 (3)	0.5022	0.0204	
akgdh	Akg_m (12345) → Suc_m (2345) + CO_2 (1)	0.4553	0.0216	
sdhf	Suc_m (1234) → Mal_m (1234)	0.4553	0.0216	0.9366
sdhs	Suc_m (1234) → Mal_m (4321)	0.6774	0.2549	
mdhf	Mal_m (1234) → Oaa_m (1234)	0.4920	0.0465	0.9493
mef	Mal_m (1234) → Pyr (123) + CO_2 (4)	-0.0367	0.0423	0.6386
pyrc	Pyr (123) + CO_2 (4) → Oaa_m (1234)	0.0602	0.0246	
pepck	Oaa_m (1234) → T3P (123) + CO_2 (4)	0.0310	0.0525	0.9218
Serf	$T3P_p$ (123) → Ser (123)	0.0116	0.0004	0.9277
Glyf	Ser (123) → Gly (12) + CHO (3)	0.0077	0.0004	0.9456
T3Ppo	$T3P_p$ →	0.0188	0.0028	
T3Po	T3P →	0.0021	0.0001	
Sero	Ser →	0.0039	0.0001	
Glyo	Gly →	0.0077	0.0004	
E4Ppo	$E4P_p$ →	0.0076	0.0023	
Pyro	Pyr →	0.0129	0.0006	
pyrpo	Pyr_p →	0.0678	0.0004	
ACApo	Aca_p →	0.2312	0.0026	
OAAmo	Oaa_m →	0.0191	0.0015	
Gluco	Akg →	0.0469	0.0036	
G6Ppout	$G6P_p$ →	0.0230	0.0020	
P5Ppout	$P5P_p$ →	0.0015	0.0004	
F6Po	F6P →	0.0195	0.0007	
CHOout	CHO →	0.0077	0.0004	

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Table S6. Metabolic network model incorporating isotopomer correction for different amino acids (Iso_corr[V]).

	Reaction	Net flux	Flux SD	Reversibility
glci	→ Glc	0.5713	0.0123	
CO2in	→ CO_{2b}	0.9024	0.0687	
CO2out	CO_2 →	3.0591	0.1274	
Alai	→ Ala	0.0002	0.0001	
Aspi	→ Asp	0.0011	0.0001	
Glui	→ Glu	0.0012	0.0001	
Glyi	→ Gly	0.0001	0.0001	
Hisi	→ His	0.0001	0.0000	
Ilei	→ Ile	0.0010	0.0001	
Meti	→ Met	0.0001	0.0001	
Seri	→ Ser	0.0007	0.0001	
Thri	→ Thr	0.0001	0.0001	
Vali	→ Val	0.0021	0.0002	
leui	→ Leu	0.0025	0.0001	
pgif	G6P (123456) → F6P (123456)	0.3924	0.0846	0.4740
g6pdh	G6P (123456) → P5P (23456)	0.1092	0.0657	
tktAf	P5P (12345) + P5P (67890) → S7P (1267890) + T3P (345)	-0.0459	0.0356	0.0880
talf	S7P (1234567) + T3P (890) → F6P (123890) + E4P (4567)	-0.0459	0.0356	0.6646
tktBf	P5P (12345) + E4P (6789) → F6P (126789) + T3P (345)	-0.0532	0.0341	0.9373
pfk	F6P (123456) → T3P (321) + T3P (456)	0.2667	0.0481	0.7474
pyrf	PEP (123) → Pyr (123)	0.8826	0.2968	
g6pt	G6P (123456) → $G6P_p$ (123456)	0.0697	0.0901	0.4748
pgifp	$G6P_p$ (123456) → $F6P_p$ (123456)	-0.7036	0.1867	0.8579
g6pdhp	$G6P_p$ (123456) → $P5P_p$ (23456) + CO_2 (1)	0.7531	0.1938	
tktAfp	$P5P_p$ (12345) + $P5P_p$ (67890) → $S7P_p$ (1267890) + $T3P_p$ (345)	0.3354	0.0757	0.9889
talfp	$S7P_p$ (1234567) + $T3P_p$ (890) → $F6P_p$ (123890) + $E4P_p$ (4567)	0.3354	0.0757	0.9687
tktBfp	$P5P_p$ (12345) + $E4P_p$ (6789) → $F6P_p$ (126789) + $T3P_p$ (345)	0.3354	0.0757	0.7960
pfkp	$F6P_p$ (123456) → $T3P_p$ (321) + $T3P_p$ (456)	0.0254	0.0554	0.1769
pepfp	$T3P_p$ (123) → Pyr_p (123)	0.2422	0.2450	
pdhp	Pyr_p (123) → Aca_p (23)	0.2266	0.0030	
t3pt	$T3P_p$ (123) → T3P (123)	0.0168	0.2477	0.1761
P5Ptf	P5P (12345) → $P5P_p$ (12345)	0.2542	0.0882	0.0422
pyrtpf	Pyr (123) → Pyr_p (123)	0.0414	0.2440	0.8668
pdh	Pyr (123) → Aca_m (23)	0.3685	0.0436	
citdh	Aca_m (12) + Oaa_m (3456) → Akg_m (65421) + CO_2 (3)	0.3685	0.0436	
akgdh	Akg_m (12345) → Suc_m (2345) + CO_2 (1)	0.3389	0.0427	
sdhf	Suc_m (1234) → Mal_m (1234)	0.3389	0.0427	0.9859
sdhs	Suc_m (1234) → Mal_m (4321)	0.6570	0.3330	
mdhf	Mal_m (1234) → Oaa_m (1234)	0.6244	0.2189	0.9337
mef	Mal_m (1234) → Pyr (123) + CO_2 (4)	-0.2856	0.1947	0.2663
pyrc	Pyr (123) + CO_2 (4) → Oaa_m (1234)	0.1722	0.2276	
pepck	Oaa_m (1234) → PEP (123) + CO_2 (4)	0.4012	0.1340	0.1748
mgdhf	Akg_m (12345) → Glu_c (12345)	0.0296	0.0023	
Serf	$T3P_p$ (123) → Ser (123)	0.0104	0.0007	
Glyf	Ser (123) → Gly (12) + CHO (3)	0.0074	0.0005	0.6071
Alaf	Pyr (123) → Ala (123)	0.0124	0.0008	
Aspf	Oaa_m (1234) → Asp (1234)	0.0148	0.0004	
Hisf	$P5P_p$ (12345) + CHO (6) → His (123456)	0.0011	0.0003	
Ilef	Thr (1234) + Pyr_p (567) → Ile (123467) + CO_2 (5)	0.0064	0.0001	
Metf	Oaa_m (1234) + CHO (5) → Met (12345)	0.0009	0.0001	
Thrf	Asp (1234) → Thr (1234)	0.0091	0.0001	
Valf	Pyr_p (123) + Pyr_p (456) → Val (12356) + CO_2 (4)	0.0239	0.0002	
Leu3f	Aca_p (12) + Val (34567) → Leu (124567) + CO_2 (3)	0.0181	0.0001	
sero	Ser →	0.0040	0.0001	

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Table S6. Metabolic network model incorporating isotopomer correction for different amino acids (Iso_corr[V]).

	Reaction	Net flux	Flux SD	Reversibility
Glyo	Gly →	0.0075	0.0005	
E4Po	E4P →	0.0073	0.0025	
pyro	Pyr →	0.0027	0.0002	
pyrpo	Pyr_p →	0.0026	0.0001	
OAAmo	Oaa_m →	0.0112	0.0011	
CHOo	CHO →	0.0054	0.0005	
Alao	Ala →	0.0127	0.0008	
Aspo	Asp →	0.0068	0.0004	
gluo	Glu →	0.0308	0.0024	
hiso	His →	0.0012	0.0003	
Ileo	Ile →	0.0074	0.0000	
Meto	Met →	0.0010	0.0001	
Thro	Thr →	0.0027	0.0000	
Valo	Val →	0.0080	0.0001	
Leuo	Leu →	0.0206	0.0001	
suco	Suc →	0.0266	0.0013	
starcho	$G6P_p$ →	0.0203	0.0022	
lipid	Aca_p →	0.2086	0.0031	

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Table S7. Metabolic network model incorporating amino acid reflux (AA_in).

	Reaction	Net flux	Flux SD	Reversibility
glci	→ Glc	0.5698	0.0105	
CO2in	→ CO_{2b}	0.1862	0.1570	
CO2out	CO_2 →	2.4669	0.1774	
CO2exf	CO_2 → CO_b	-0.1429	0.1573	0.7763
Alai	→ Ala	0.0018	0.0017	
Aspi	→ Asp	0.0016	0.0004	
Glui	→ Glu	0.0011	0.0012	
Glyi	→ Gly	0.0003	0.0003	
Hisi	→ His	0.0001	0.0000	
Ilei	→ Ile	0.0008	0.0001	
Meti	→ Met	0.0001	0.0001	
Seri	→ Ser	0.0007	0.0003	
Thri	→ Thr	0.0003	0.0001	
Vali	→ Val	0.0016	0.0004	
leui	→ Leu	0.0019	0.0001	
Pyrpi	→ Pyr_p	0.0008	0.0002	
Oaami	→ Oaa_m	0.0025	0.0015	
Pyri	→ Pyr	0.0009	0.0004	
Suci	→ Suc_m	0.0078	0.0013	
Starchi	→ $G6P_p$	0.0044	0.0006	
T3Ppi	→ $T3P_p$	0.0024	0.0012	
E4Ppi	→ $E4P_p$	0.0014	0.0008	
Acapi	→ Aca_p	0.0094	0.0011	
Acain	→ Aca_1	0.0083	0.0031	
Acatf	Aca_1 (123)→ Aca_m (123)	0.0083	0.0031	
pgif	G6P (123456) → F6P (123456)	0.3577	0.1008	0.3712
g6pdh	G6P (123456) → P5P (23456)	0.1651	0.0709	
tktAf	P5P (12345) + P5P (67890) → S7P (1267890) + T3P (345)	-0.0130	0.0647	0.3276
talf	S7P (1234567) + T3P (890) → F6P (123890) + E4P (4567)	-0.0130	0.0647	0.7689
tktBf	P5P (12345) + E4P (6789) → F6P (126789) + T3P (345)	-0.0184	0.0647	0.7768
pfk	F6P (123456) → T3P (321) + T3P (456)	0.3071	0.0659	0.5756
pyrf	PEP (123) → Pyr (123)	0.8414	0.2060	
g6pt	G6P (123456) → $G6P_p$ (123456)	0.0470	0.0591	0.2965
pgifp	$G6P_p$ (123456) → $F6P_p$ (123456)	-0.4002	0.2359	0.8545
g6pdhp	$G6P_p$ (123456) → $P5P_p$ (23456) + CO_2 (1)	0.4301	0.2293	
tktAfp	$P5P_p$ (12345) + $P5P_p$ (67890) → $S7P_p$ (1267890) + $T3P_p$ (345)	0.2128	0.1120	0.9950
talfp	$S7P_p$ (1234567) + $T3P_p$ (890) → $F6P_p$ (123890) + $E4P_p$ (4567)	0.2128	0.1120	0.9847
tktBfp	$P5P_p$ (12345) + $E4P_p$ (6789) → $F6P_p$ (126789) + $T3P_p$ (345)	0.2128	0.1120	0.8536
pfkp	$F6P_p$ (123456) → $T3P_p$ (321) + $T3P_p$ (456)	0.0254	0.0554	0.3931
pepfp	$T3P_p$ (123) → Pyr_p (123)	0.1374	0.1409	
pdhp	Pyr_p (123) → Aca_p (23)	0.2164	0.0033	
t3pt	$T3P_p$ (123) → T3P (123)	0.1159	0.1636	0.0944
P5Ptf	P5P (12345) → $P5P_p$ (12345)	0.2096	0.1437	0.0481
pyrtpf	Pyr (123) → Pyr_p (123)	0.1601	0.1471	0.7409
pdh	Pyr (123) → Aca_m (23)	0.4844	0.0616	
citdh	Aca_m (12) + Oaa_m (3456) → Akg_m (65421) + CO_2 (3)	0.4927	0.0627	
akgdh	Akg_m (12345) → Suc_m (2345) + CO_2 (1)	0.4623	0.0626	
sdhf	Suc_m (1234) → Mal_m (1234)	0.4735	0.0586	0.9596
sdhs	Suc_m (1234) → Mal_m (4321)	0.3905	0.3322	
mdhf	Mal_m (1234) → Oaa_m (1234)	0.4902	0.1463	0.9339
mef	Mal_m (1234) → Pyr (123) + CO_2 (4)	-0.0167	0.1329	0.3278
pyrc	Pyr (123) + CO_2 (4) → Oaa_m (1234)	0.1676	0.1103	
pepck	Oaa_m (1234) → PEP (123) + CO_2 (4)	0.1410	0.0875	0.1850
mgdhf	Akg_m (12345) → Glu_c (12345)	0.0303	0.0026	0.7068

Electronic Supplementary Material (ESI) for Molecular BioSystems

Supplementary Tables

Table S7. Metabolic network model incorporating amino acid reflux (AA_in).

	Reaction	Net flux	Flux SD	Reversibility
Serf	$T3P_p$ (123) → Ser (123)	0.0104	0.0007	0.5454
Glyf	Ser (123) → Gly (12) + CHO (3)	0.0072	0.0006	0.7329
Alaf	Pyr (123) → Ala (123)	0.0109	0.0017	0.8792
Aspf	Oaa_m (1234) → Asp (1234)	0.0144	0.0005	0.3232
Hisf	$P5P_p$ (12345) + CHO (6) → His (123456)	0.0012	0.0003	
Ilef	Thr (1234) + Pyr_p (567) → Ile (123467) + CO_2 (5)	0.0066	0.0001	
Metf	Oaa_m (1234) + CHO (5) → Met (12345)	0.0009	0.0001	
Thrf	Asp (1234) → Thr (1234)	0.0090	0.0001	
Valf	Pyr_p (123) + Pyr_p (456) → Val (12356) + CO_2 (4)	0.0363	0.0090	
Valcat	Val (12345) → Suc_m (2345) + CO_2 (1)	0.0112	0.0094	
Leu3f	Aca_p (12) + Val (34567) → Leu (124567) + CO_2 (3)	0.0187	0.0002	
sero	Ser →	0.0039	0.0001	
Glyo	Gly →	0.0075	0.0004	
E4Po	E4P →	0.0067	0.0021	
pyro	Pyr →	0.0026	0.0002	
pyrpo	Pyr_p →	0.0026	0.0001	
OAAmo	Oaa_m →	0.0113	0.0009	
CHOo	CHO →	0.0050	0.0007	
Alao	Ala →	0.0127	0.0006	
Aspo	Asp →	0.0070	0.0003	
gluo	Glu →	0.0314	0.0022	
hiso	His →	0.0013	0.0003	
Ileo	Ile →	0.0075	0.0001	
Meto	Met →	0.0010	0.0001	
Thro	Thr →	0.0026	0.0001	
Valo	Val →	0.0080	0.0001	
Leuo	Leu →	0.0206	0.0001	
suco	Suc →	0.0270	0.0014	
starcho	$G6P_p$ →	0.0215	0.0019	
lipid	Aca_p →	0.2071	0.0030	