

Supplemental Data for:

Haggerty JJ, Taylor DK and Jiranek V. 2016.

Monitoring volatile aroma compounds during fermentation in a chemically defined grape juice medium deficient in leucine.

Am J Enol Vitic 67:350-356. doi: 10.5344/ajev.2016.15026.

Supplemental Table 1 Composition of model media for MS300 (Rossouw and Bauer 2009) and CDGJM (Henschke and Jiranek 1993). (Assimilable nitrogen was calculated as total nitrogen content excluding that from proline.)

Component	MS300	CDGJM	Component	MS300	CDGJM
pH (NaOH)	3.3	3.23.5	Vitamins	(mg/L)	(mg/L)
			Myoinositol	20	100
Sugars	(g/L)	(g/L)	Nicotinic acid	2	2
Glucose	125	100	Calcium pantothenate	1.5	1
Fructose	125	100	Thiamine HCl	0.25	0.5
			Pyridoxine HCl	0.25	2
Amino acids	(mg/L)	(mg/L)	Biotin	0.003	0.125
Alanine	145.3	100	pAminobenzoic acid		0.2
Arginine	374.4	750	Riboflavin		0.2
Asparagine		150	Folic acid		0.2
Aspartic acid	44.5	350			
Cysteine	13.1		Mineral salts	(mg/L)	(mg/L)
Glutamic acid	120.4	500	K ₂ SO ₄	500	
Glutamine	505.3	200	NaCl	200	
Glycine	18.3	50	MnSO ₄ ·H ₂ O	4	
Histidine	32.7	150	ZnSO ₄	4	
Isoleucine	32.7	200	CuSO ₄ ·5H ₂ O	1	
Leucine	48.4	300	KI	1	
Lysine	17.0	250	CoCl ₂ ·6H ₂ O	0.4	
Methionine	31.4	150	KH ₂ PO ₄	750	1140
Phenylalanine	37.9	150	MgSO ₄ ·7H ₂ O	250	1230
Proline	612.6	500	CaCl ₂ ·2H ₂ O	155	440
Serine	78.5	400	H ₃ BO ₃	1	0.0057
Threonine	759.3	350	NaMoO ₄ ·2H ₂ O	1	0.0242
Tryptophan	179.3	100	Co(NO ₃) ₂ ·6H ₂ O		0.0291
Tyrosine	18.3	20	CuCl ₂		0.0136
Valine	44.5	200	FeCl ₂		0.0320
Total amino acids	3113.9	4870	ZnCl ₂		0.1355
Assimilable nitrogen (mg N/L)	419	723	KIO ₃		0.0108
Ammonium chloride	460	100	K tartrate		5000
Total assimilable nitrogen (mg N/L)	537	749	L-Malic acid		3000
			Citric acid		200
			MnCl ₂ ·4H ₂ O		0.1982

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Supplemental Table 2 Aroma compounds formed by *Saccharomyces cerevisiae* with odor activity values greater than 1.

Compound	Aroma description	Odor threshold ($\mu\text{g/L}$)
Ethyl esters		
ethyl acetate	pineapple, fruity, solvent	7500
ethyl 2-methylpropanoate	sweet, rubber	15
ethyl 2-methylbutanoate	apple	18/1
ethyl 3-methylbutanoate	fruit	3
ethyl butanoate	apple	20
ethyl hexanoate	apple peel, fruit	14/5
ethyl octanoate	fruit, fat	2
ethyl decanoate	grape	200
ethyl lactate	fruit	14
ethyl dodecanoate	soapy, estery	-
ethyl propanoate	fruity	1800
Acetates		
3-methylbutyl acetate	banana	30
2methylbutyl acetate	fruit	160
2-phenylethyl acetate	rose, honey, tobacco	250
hexyl acetate	fruit, herb	670
2-methylpropyl acetate	fruit, apple, banana	1.6
Acids		
2-methylpropanoic acid	rancid, butter, cheese	2300
3-methylbutanoic acid	sweat, acid, rancid	33.4
acetic acid	sour	200,000
2-methylbutanoic acid	cheese, sweaty	1500
butanoic acid	rancid, cheese, sweat	173
hexanoic acid	sweat	420
octanoic acid	sweat, cheese	500
decanoic acid	rancid, fat	1000/8100
Alcohols		
benzyl alcohol	sweet, flower	900,000
butanol	wine, fusel, spiritous	150,000
2-methyl propanol	wine, solvent, bitter	40,000
3-methyl butanol	whisky, malt, burnt	30,000
2methyl butanol	wine, onion	65,000
2phenyl ethanol	honey, spice, rose, lilac	14,000/10,000
methionol	sweet potato	1000
<i>n</i> -propanol	alcohol, pungent	306,000
2,3-butanediol	fruity	150,000
hexanol	resin, flower, green	8000
Miscellaneous		
2,3-butanedione	butter	100

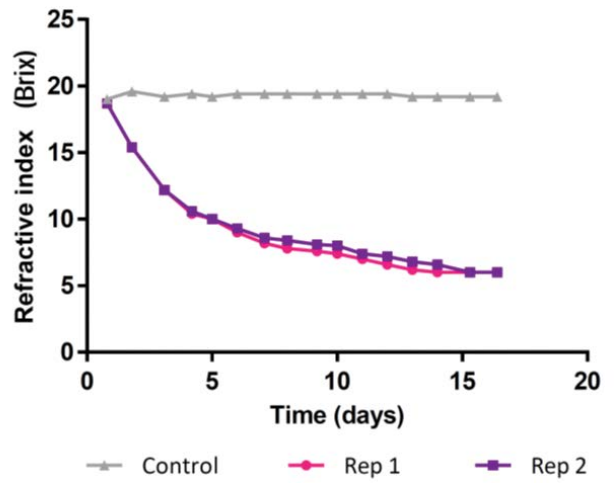
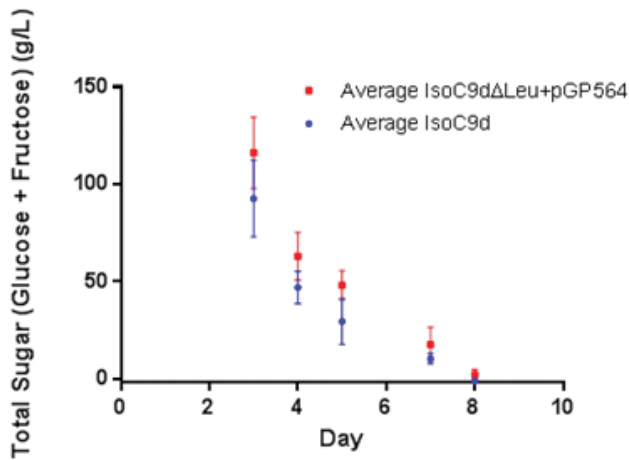
Aroma descriptors are from Flavournet (Acree and Arn 2004); odor thresholds determined in ~10% ethanol (Francis and Newton 2005, Ferreira et al. 2000, Guth 1997, Peinado et al. 2006, Peinado et al. 2004, Salo 1970, Siebert et al. 2005).

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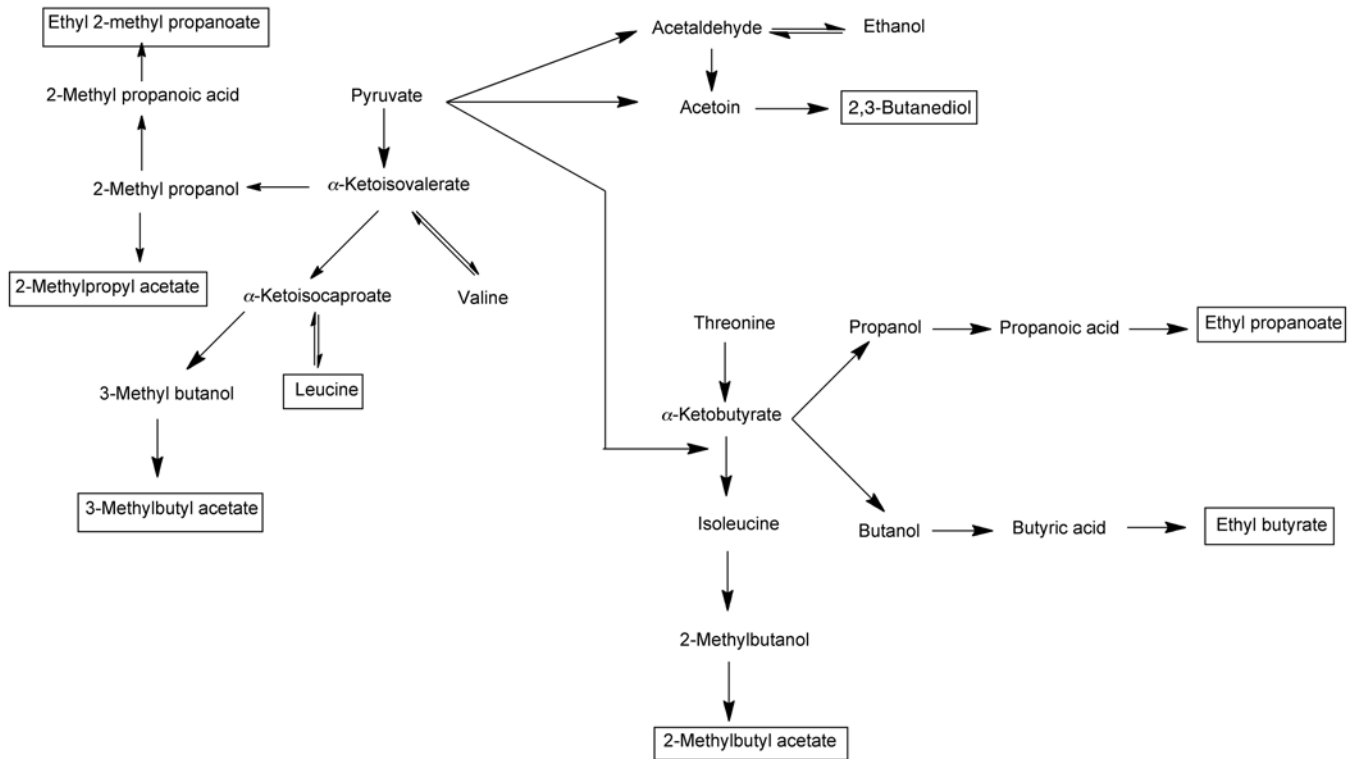
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Supplemental Figure 1 Fermentation kinetics of strains isoC9D and iso-C9DΔLEU+pGP564 grown in CDGJM lacking leucine. Fermentations were conducted in deep-well (~2 mL) plates and are reported as averages for each time point (n = 40).

Supplemental Figure 2 Fermentation curve for replicate 1, replicate 2 of strain iso-C9DΔLEU+pGP564, and the uninoculated control, as measured by refractometry in Brix.



Supplemental Figure 3 A simplified version of the pathways involved in the production of the aroma compounds linked to leucine biosynthesis (Baichwal et al. 1983, Bollon 1974, González et al. 2000, Guymon et al. 1961, Hazelwood et al. 2008, Ingraham et al. 1961).

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