

Table S1. Deuterated internal standards used for determination of fermentation volatiles by GC-MS.

Analyte	RT (min)	Ions ¹ (m/z)	Internal standard
ethyl acetate	6.783	61 , 70, 88	d ₈ -ethyl acetate
ethyl propanoate	8.492	75, 80, 102	d ₅ -ethyl propanoate
ethyl 2-methylpropanoate	8.712	88,101, 116	d ₅ -ethyl 2-methyl propanoate
2-methylpropyl acetate	10.107	56 , 73, 86	d ₉ -2-methylpropyl acetate
ethyl butanoate	10.870	71, 88, 101	d ₅ -ethyl butanoate
ethyl 2-methylbutanoate	11.375	85, 102 , 115	d ₅ -ethyl 2-methyl butanoate
ethyl 3-methylbutanoate	11.872	85, 88 , 115	d ₅ -ethyl 2-methyl butanoate
2-methyl-1-propanol	12.781	41, 43 , 74	d ₉ -2-methyl-1-propanol
2-methylbutyl acetate	13.681	57, 72, 74	d ₉ -3-methylbutyl acetate
3-methylbutyl acetate	13.718	55, 87, 88	d ₉ -3-methylbutyl acetate
1-butanol	14.473	41, 44, 56	d ₁₀ -1-butanol
2-methyl-1-butanol	16.522	41, 56, 70	d ₉ -3-methyl-1-butanol
3-methyl-1-butanol	16.522	55, 60, 70	d ₉ -3-methyl-1-butanol
ethyl hexanoate	17.419	88 , 99, 115	d ₅ -ethyl hexanoate
hexyl acetate	18.692	69, 73, 84	d ₁₃ -hexyl acetate
hexanol	21.018	55, 56 , 69	d ₁₃ -hexanol
ethyl octanoate	23.441	88, 101 , 127	d ₅ -ethyl octanoate
acetic acid	24.058	43, 60	d ₃ -acetic acid
propanoic acid	26.283	57, 73, 74	d ₅ -propanoic acid
2-methylpropanoic acid	26.979	43, 73 , 88	d ₇ -2-methylpropanoic acid
butanoic acid	28.553	45, 60 , 73	d ₇ -butanoic acid
ethyl decanoate	28.811	101, 157, 200	d ₅ -ethyl decanoate
3-methylbutanoic acid	29.686	60 , 61	d ₇ -3-methylbutanoic acid
2-methylbutanoic acid	29.704	57, 74	d ₇ -3-methylbutanoic acid
2-phenylethyl acetate	33.010	65, 91, 104	d ₃ -2-phenylethyl acetate
hexanoic acid	33.435	60 , 73, 87	d ₁₁ -hexanoic acid
2-phenylethanol	34.667	91 , 92, 122	d ₃ -2-phenylethanol
octanoic acid	36.641	60, 85, 115	d ₁₅ -octanoic acid
decanoic acid	39.304	73, 129 , 172	d ₁₉ -decanoic acid

¹ The bolded ion was used for quantification.


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