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Supplemental Information

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The generation characteristics and spreading risk of VOCs released

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from a biological fermentation pharmaceutical factory

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17 Table S1 Classification of gases detected during fermentation (VOCs: Volatile
 18 organic compounds)

Species	Composition
Chlorine-containing organics (15.11%)	1-Chloro-2-methylpropane, 2-Chloro-2-methylpropane, Allyl Chloride, Carbon Tetrachloride, Chloroform, Dichloromethane, Trichloroacetic Acid
Nitrogen-containing organics (19.93%)	1-Methyl-2-pyrrolidinone, Diethylamine, N- Nitrosodibutylamine, N-Nitrosodiethylamine, Dimethylhydrazine
VOCs (95.76%)	Propylene Oxide, 1-Heptaldehyde, Acetaldehyde, Hexanaldehyde, Propanal, Butyraldehyde, Crotonaldehyde, 2-Pentanone, Methyl ethyl ketone, Dimethyl heptanone, Butyl Acetate, Methyl Cellosolve Acetate, Vinyl Acetate, methanol
Oxygen-containing organics (40.73%)	
Aromatic hydrocarbon compounds (13.35%)	Benzene, Indene, O-Xylene, Phenol, Chlorobenzene
Phosphorous organics (3.55%)	Trimethyl Phosphite
Sulfur-containing organics (2.20%)	Sulfuryl Fluoride, Thionyl Fluoride, Sulfur Hexafluoride
Alkane (0.88%)	Ethane, Cyclohexane
Inorganic compounds (4.24%)	SO ₂ F ₂ , N ₂ O, NO ₂ , SOF ₂ , NH ₃ , HCN, CO, SO ₂

- 21 Table S2 Parameters and reference value used for risk assessment of VOCs (VOCs:
 22 Volatile organic compounds, CASRN: Chemical abstracts service registry number,
 23 Group: Group of carcinogens by the International Agency for Research on Cancer,
 24 Group 1: Carcinogenic to humans, Group 2A: Probably carcinogenic to humans,
 25 Group 2B: Possibly carcinogenic to humans.)

Parameter	Units	Values		
		Adult male	Adult female	
Time for exposure(Te)	h/d	8	8	
Duration for exposure(De)	yr	30	30	
Annual exposure frequently(AEF)	d/yr	250	250	
Average lifetime(AT)	h	$72.4 \times 365 \times 24$	$77.4 \times 365 \times 24$	
VOCs	CASRN	Group	Inhalation unit risk(IUR)[(ug/m ³) ⁻¹]	Source
Benzene	71-43-2	1	7.8×10^{-6}	IRIS
Dichloromethane	75-09-2	2A	1×10^{-8}	IRIS
Acetaldehyde	75-07-0	2B	2.2×10^{-6}	IRIS
Propylene Oxide	75-56-9	2B	3.7×10^{-6}	IRIS
Carbon Tetrachloride	56-23-5	2B	6×10^{-6}	IRIS

Table S3 Olfactory effect analysis (OT_i: odour detected threshold of compound i (mg/m³), OAV_i: odour activity value of compound i, PO_i: odour contribution rate of compound i, TOAV: total odour activity value, (10 hours, 60 hours, 110 hours, 160 hours, 200 hours, 240 hours mean different fermentation time in a complete fermentation cycle.)

compounds	OT _i (mg/m ³)	10 h		60 h		110 h		160 h		200 h		240 h	
		OAV _i	PO _i (%)	OAV _i	PO _i (%)	OAV _i	PO _i (%)	OAV _i	PO _i (%)	OAV _i	PO _i (%)	OAV _i	PO _i (%)
Carbon	28.91	5.17	0.02%	0.58	0.00%								
Tetrachloride													
Chloroform	18.46	2.62	0.01%										
Dichloromethane	555.10	0.86	0.00%										
Diethylamine	0.14	67.71	0.20%									2030	37.11%
Acetaldehyde	0.0027	18594.24	55.69%	18594.24	76.61%			71740	99.10%	12006.67	59.33%		
Propanal	0.0024	12860	38.51%										
Butyraldehyde	0.0020					10537.31	99.59%			7641.79	37.76%	3432.84	62.76%

Crotonaldehyde	0.066	417.39	1.25%	285.47	1.18%			589.13	0.81%	544.78	2.69%		
Methyl ethyl ketone	1.29	215.43	0.65%										
Butyl Acetate	0.076	1070	3.20%	2591.7 4	10.68%								
Benzene	8.60	14.76	0.04%			17.38	0.16%	13.88	0.02%	14.76	0.07%	7.30	0.13%
o-Xylene	1.64			9.43	0.04%			29.68	0.04%	29.74	0.15%		
Phenol	0.021	142.86	0.43%	2756.7 3	11.36%								
Carbon Disulfide	0.65			31.76	0.13%	19.76	0.19%	17.62	0.02%				
Carbonyl Sulfide	0.13												
Cyclohexane	8.57			0.13	0.00%	5.81	0.05%						
TOAV		33391.		24270.		10580.2		72390.		20237.7			5470.14
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Table S4 Cancer risk of the health-related VOCs (Rt: total carcinogenic risk. (10 hours, 60 hours, 110 hours, 160 hours, 200 hours, and 240 hours mean different fermentation times in a complete fermentation cycle.)

Time		Benzene	Dichloromethane	Acetaldehyde	Propylene Oxide	Carbon Tetrachloride	Rt
10 h	Meal	9.36×10^{-5}	4.51×10^{-7}	4.47×10^{-6}	7.08×10^{-6}	8.51×10^{-5}	1.91×10^{-4}
	Female	8.76×10^{-5}	4.22×10^{-7}	4.19×10^{-6}	6.63×10^{-6}	7.63×10^{-5}	1.75×10^{-4}
60 h	Male	0	0	1.04×10^{-5}	0	9.60×10^{-6}	2.00×10^{-5}
	Female	0	0	9.75×10^{-6}	0	8.98×10^{-6}	1.87×10^{-5}
110 h	Male	1.10×10^{-4}	0	0	0	0	1.10×10^{-4}
	Female	1.03×10^{-4}	0	0	0	0	1.03×10^{-4}
160 h	Male	8.81×10^{-5}	0	4.02×10^{-5}	1.12×10^{-5}	0	1.40×10^{-4}
	Female	8.24×10^{-5}	0	3.76×10^{-5}	1.05×10^{-5}	0	1.31×10^{-4}
200 h	Male	9.36×10^{-5}	0	6.73×10^{-6}	6.62×10^{-6}	0	1.07×10^{-4}
	Female	8.76×10^{-5}	0	6.30×10^{-6}	6.19×10^{-6}	0	1.00×10^{-4}
240 h	Male	4.63×10^{-5}	0	0	0	0	4.63×10^{-5}
	Female	4.33×10^{-5}	0	0	0	0	4.33×10^{-5}