

Supporting Information for
Indicator of harmful cyanobacteria using an odor-binding protein-
based biosensor for β -cyclocitral detection

Chunmiao Wang^{1,2}, Xinying Chang³, Zhenao Gu^{2,4}, Yaohan Qian^{1,2}, Wanqing Liu¹,
Anqi Jia¹, Zhugen Yang⁵, Jianwei Yu^{2,3*}, Min Yang^{1,2*}

¹ National Engineering Research Center of Industrial Wastewater Detoxication and Resource Recovery, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing 100085, China;

² University of Chinese Academy of Sciences, Beijing, 100049, China;

³ Beijing Drainage Group Co. Ltd (BDG), Beijing, 100124, China;

⁴ Key Laboratory of Environmental Aquatic Chemistry, State Key Laboratory of Regional Environment and Sustainability, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing, 100085, China;

⁵ Faculty of Engineering and Applied Sciences, Cranfield University, Cranfield MK43 0AL, UK.

*Corresponding author:

E-mail: jwyu@rcees.ac.cn; Tel: 86-10-62849149; Fax: 86-10-62923541;

E-mail: yangmin@rcees.ac.cn; Tel: 86-10-62923475; Fax: 86-10-62923541.

Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing, 100085, China.

Pages	1-8
Table	S1-S4
Figures	S1-S4

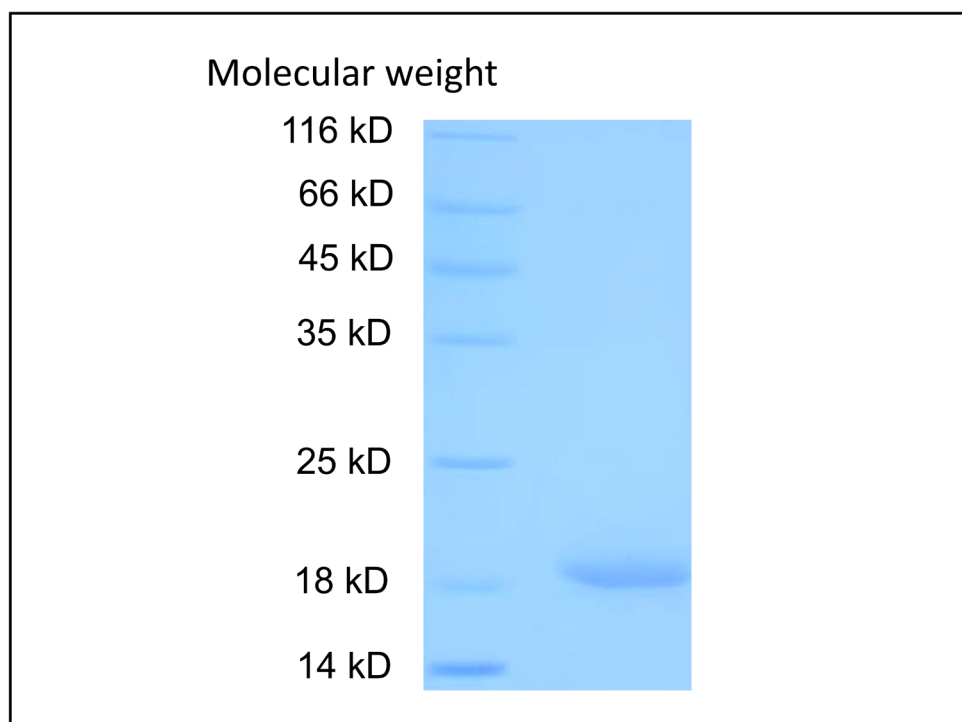
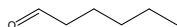
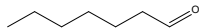
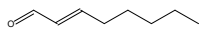
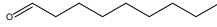
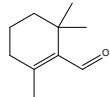
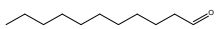
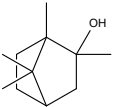
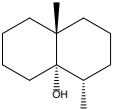
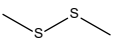
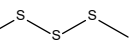


Fig. S.1 SDS-PAGE analysis of recombinant OBP2a

Table S.1 The detailed information for the 10 odorants (Guo et al. 2023, Wang et al. 2021)

Odorants	Structures	CAS	MW <i>a</i>	Catalogue number	Reagent brand	OTC ^c (µg/L)	odor descriptors	Concentrations in finished water (ng/L)	detection frequency (%)	
Aldehyde	Hexanal		66-25-1	100.2	IST00097 7-1ml	Alta	0.3 – 14	grassy/ fatty	n.d.-243	79
	Heptanal		111-71-7	114.2	m-554-07	Accustan- dard	3	fishy/fatty	n.d.-578	42
	2-Octenal		2548-87-0	126.2	52464	Supelco	3	fishy	n.d.-34.5	1.4
	Decanal		112-31-2	156.3	71441- 10mg	TMstand- ard	0.8	fruity	n.d.-153	35
	β-Cyclocitral		432-25-7	152.2	16976	Supelco	19.3	grassy/swe- et-tobacco	n.d.-57.4	32
	Undecanal		112-44-7	170.3	CCEM500 747	CATO	0.55	fatty/fruity	800	-

Odorants		Structures	CAS	MW ^a	Catalogue number	Reagent brand	OTC ^c (µg/L)	odor descriptors	Concentrations in finished water (ng/L)	detection frequency (%)
Terpene	2-Methylisoborneol		2371-42-8	168.2	DRE-LA150884-00ME	Dr.Ehrenstorfer	0.010	musty/earthy	n.d.-576	36
	Geosmin		19700-21-1	182.3	G5908-1ML	Supelco	0.004	musty/earthy	n.d.-10	50
Thioether	Dimethyl disulfide		624-92-0	94.2	BePure-22165	Bepure	0.030	swampy/septic	n.d.-8.7	45
	Dimethyl trisulfide		3658-80-8	126.3	1ST2941-100mg	Alta	0.010	swampy/septic	n.d.-3.3	25

Note: ^a Molecular weight; ^b Octanol-Water Partition Coefficient; ^c odor threshold concentration.

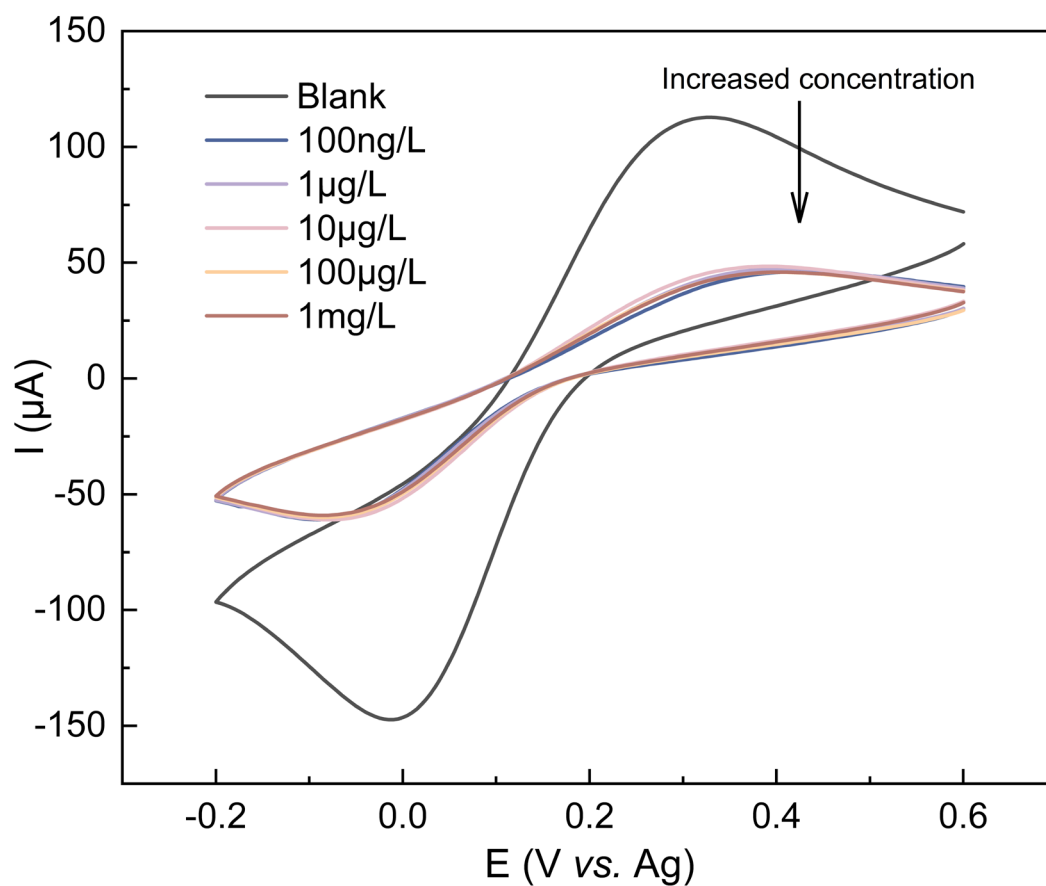


Fig. S.2 Cyclic voltammetry detection results of β -cyclocitral by the bare SPE

Table S.2 Dissociation constants (K_i) and molecular docking results for 10 odorants

Odorant	Docking socre	K_i
Hexanal	-3.92	41.49 ± 0.39
Heptanal	-4.36	43.87 ± 0.25
2-Octenal	-4.73	29.91 ± 0.15
Decanal	-4.15	31.59 ± 0.13
β -Cyclocitral	-6.61	34.79 ± 2.36
Undecanal	-3.7	61.05 ± 1.53
2-MIB	-3.8	43.89 ± 0.17
GSM	-4.69	63.06 ± 0.01
DMDS	-3.04	50.72 ± 0.31
DMTS	-4.19	41.83 ± 0.13

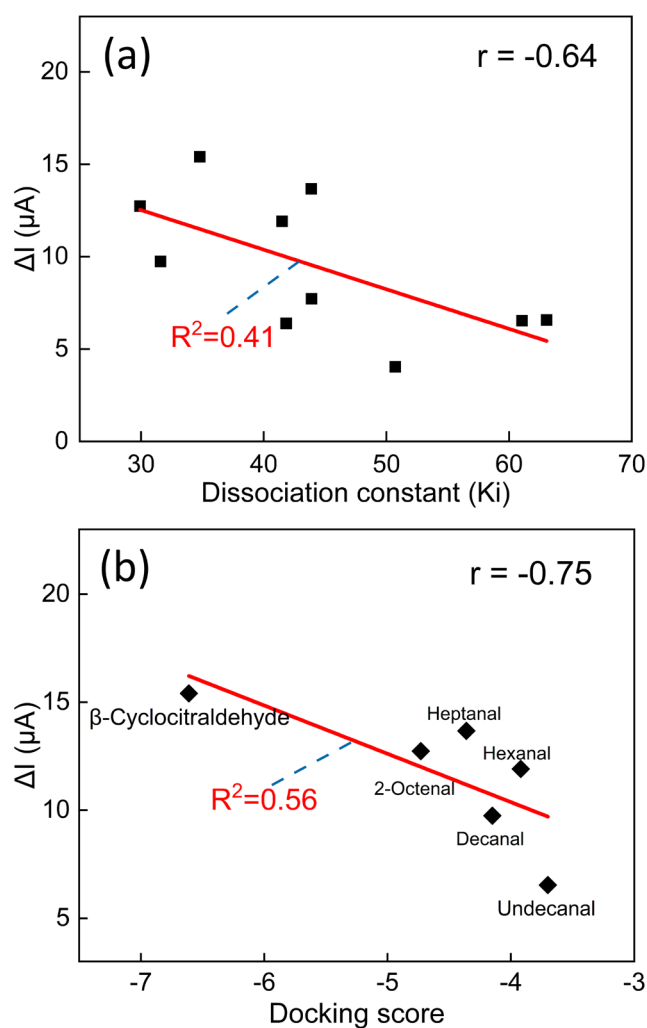


Fig. S.3 Correlation analysis of dissociation constants (K_i) and ΔI of 10 odorants (a); Relation of docking score with ΔI of aldehydes (b).

Table S.3 Average recovery of different concentrations of β -cyclocitral

Spiked	Recovery rate (%)	RSD (%)
200ng/L	116.82	6.29
5 μ g/L	95.41	13.54
50 μ g/L	91.69	8.12

Note: n=3.

Table S.4 Results for the detection of odorants in the raw water

Number	Odorant	Detection result (ng/L)
1	2-MIB	n.d.
2	Geosmin	10.25
3	DMDS	n.d.
4	DMTS	11.04
5	Hexanal	3.66
6	Benzaldehyde	82.80
7	Undecanal	52.68
8	β -Cyclocitral	8.83
9	2E4MDL	8.84
10	DCIP	81.57

Note: n.d.: Not detected.

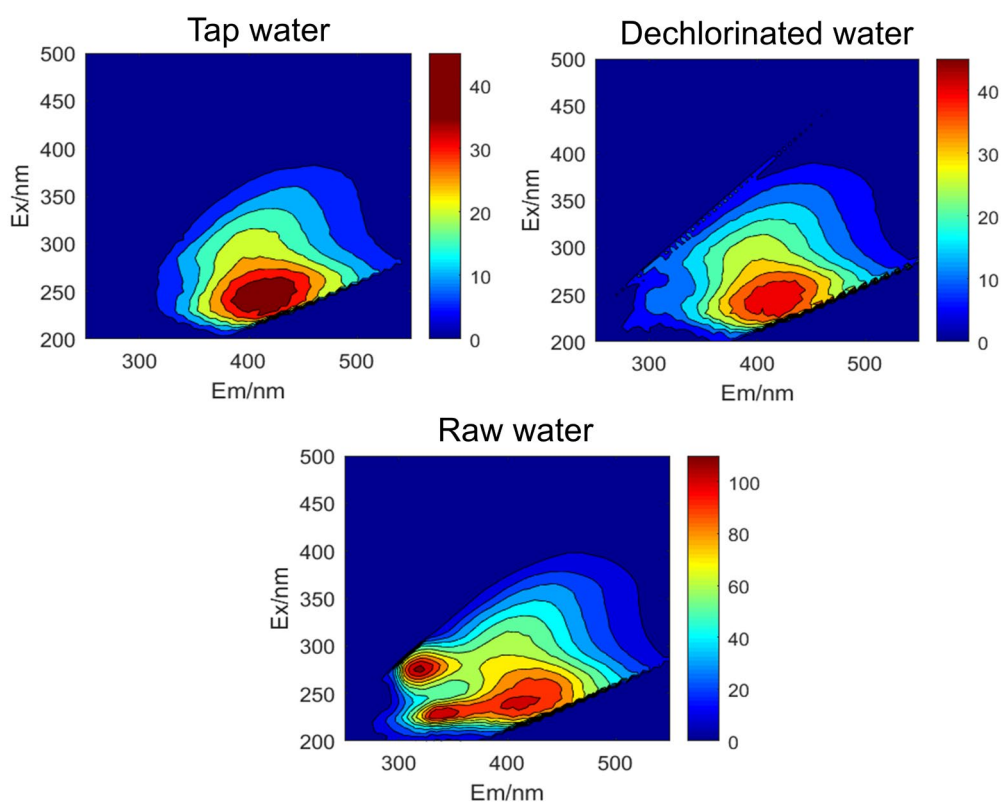


Fig. S.4 Analysis of organic matter fractions in different matrices

Reference

Guo, Q., Chen, X., Yang, K., Yu, J., Liang, F., Wang, C., Yang, B., Chen, T., Li, Z., Li, X. and Ding, C. (2023) Identification and evaluation of fishy odorants produced by four algae separated from drinking water source during low temperature period: Insight into odor characteristics and odor contribution of fishy odor-producing algae. *Chemosphere* 324, 138328.

Wang, C., Gallagher, D.L., Dietrich, A.M., Su, M., Wang, Q., Guo, Q., Zhang, J., An, W., Yu, J. and Yang, M. (2021) Data Analytics Determines Co-occurrence of Odorants in Raw Water and Evaluates Drinking Water Treatment Removal Strategies. *Environ Sci Technol* 55(24), 16770-16782.



DSPACE

<https://dspace.org/>

Indicator of harmful cyanobacteria using an odor-binding protein-based biosensor for -cyclocitral detection

Wang, Chunmiao; Chang, Xinying; Gu, Zhenao; Qian, Yaohan; Liu, Wanqing ...

2026-05

Elsevier

<https://doi.org/10.1016/j.jwpe.2026.110122>

Wang C, Chang X, Gu Z, et al., (2026) Indicator of harmful cyanobacteria using an odor-binding protein-based biosensor for -cyclocitral detection. Journal of Water Process Engineering, Volume 87, May 2026, Article number 110122