

Supplementary Material

Text S1. Classification of the assigned molecules in the van Krevelen (V-K) diagram.

The assigned molecules are distinguished from the various compounds in the V-K diagram through H/C and O/C cutoffs. we divided the V-K diagram into seven regions, representing the seven compounds in DOM. The seven classes of various compounds were described as follows: aliphatic/proteins ($1.5 \leq \text{H/C} \leq 2.2$, $0.3 \leq \text{O/C} \leq 0.67$), lipids ($1.5 \leq \text{H/C} \leq 2.0$, $0 \leq \text{O/C} \leq 0.3$), lignins/CRAM-like structures ($0.7 \leq \text{H/C} \leq 1.5$, $0.1 \leq \text{O/C} \leq 0.67$), unsaturated hydrocarbons ($0.7 \leq \text{H/C} \leq 1.5$, $0 \leq \text{O/C} \leq 0.1$), carbohydrates ($1.5 \leq \text{H/C} \leq 2.4$, $0.67 \leq \text{O/C} \leq 1.2$), aromatic structures ($0.2 \leq \text{H/C} \leq 0.7$, $0 \leq \text{O/C} \leq 0.67$), and tannins ($0.6 \leq \text{H/C} \leq 1.5$, $0.67 \leq \text{O/C} \leq 1.2$).

Table S1. Basic water quality index testing of chemical industry park tailwater.

Name	Value / Range	Unit
pH	(7.9 ± 0.2)	-
Colour	(672.7 ± 80.6)	Hazen
Turbidity	(471.7 ± 65.3)	NTU
COD	(270.5 ± 62.1)	mg/L
Cl ⁻	>10000	mg/L
B/C	(0.29 ± 0.2)	-
NH ₄ ⁺ -N	(17.8 ± 9.7)	mg/L
NO ₃ ⁻ -N	(33.1 ± 4.5)	mg/L
TN	(59.2 ± 16.1)	mg/L

Note: All indicators were collected from the tailwater of the chemical industrial park and tested using a portable water quality detector.



Table S2. Effluent quality comparison of SCOB, Ozone, and Bio treatment under stable operational phase (Stage III).

Name (Unit)	Inf	SCOB	Ozone	Bio
COD (mg/L)	(270.5 ± 62.1)	(98.3 ± 49.3)	(124.0 ± 47.9)	(193.5 ± 38.9)
Colour (Hazen)	(672.7 ± 80.6)	(84.5 ± 55.6)	(173.3 ± 74.5)	(442.8 ± 43.2)
Turbidity (NTU)	(471.7 ± 65.3)	(29.7 ± 9.4)	(57.0 ± 18.6)	(133.5 ± 27.4)
SO ₄ ²⁻ (mg/L)	(3649.9 ± 112.2)	(5914.6 ± 117.1)	(4942.7 ± 342.7)	(4305.6 ± 171.7)
UV ₂₅₄	(2.5 ± 0.06)	(0.26 ± 0.007)	(0.39 ± 0.002)	(2.08 ± 0.05)