Managing Disinfection and By-products for Safe Water

24 APRIL 2024

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AGENDA

- **Introduction**
  Xin Gao, Xylem/Management Committee member, Disinfection SG
- **Should aromatic DBPs be managed as a priority?**
  Mengting Yang, Shenzhen University, China
- **Understanding the Radical Involved Reactions of Dissolved Organic Matter: Kinetics and DBP Formation**
  Xin Yang, Sun Yat-sen University, China
- **Q&A Panel Discussion**
  Speakers and Moderator
- **Close**
  Xin Gao, Xylem/Management Committee member, Disinfection SG

WEBINAR INFORMATION

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- This webinar will be **recorded and made available "on-demand"** on the IWA Connect Plus platform and IWA Network website, with presentation slides, and other information.
- The **speakers** are responsible for **securing copyright permissions** for any work that they will present of which they are not the legal copyright holder.
- The opinions, hypothesis, conclusions or recommendations contained in the presentations and other materials are the **sole responsibility of the speaker(s)** and do not necessarily reflect IWA opinion.

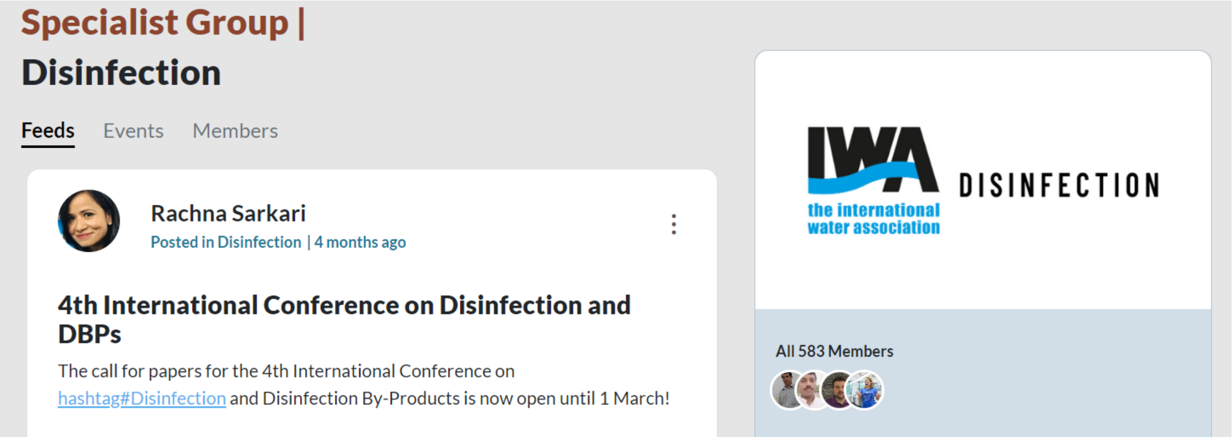
WEBINAR INFORMATION

- **‘Chat’ box**: please use this for general requests and for interactive activities.
- **‘Q&A’ box**: please use this to send questions to the panelists.
  (We will answer these during the discussions)

Please Note: *Attendees’ microphones are muted. We cannot respond to ‘Raise Hand’.*

ABOUT DISINFECTION SG

- The Disinfection SG aims to create, exchange and transfer the knowledge and experience of disinfection-related issues in water, wastewater, sludge or excreta.
- The Disinfection SG strategic plan includes reinvigorating its membership participation, encouraging the exchange of knowledge and inspiring the collaboration between water industries, academia, government and public.
- The group encourages achievements in disinfection to include practical solutions for the low-income countries as well as leading-edge technologies and theories.



https://www.iwaconnectplus.org/group/feeds?CommunityKey=a0M4K0000027gbZUAQ

NEXT CONFERENCE: 4TH IWA D&DBPS CONFERENCE

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UNIVERSIDAD DE ALMERÍA

CIESOL Solar Energy Research Center Joint Center UAL - PSA CIEMAT

Ciemat PSA

ALMERÍA CIUDAD

21 – 24 October 2024 | Almeria, Spain

SPEAKERS

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Xin Yang
Sun Yat-sen University,
China

Mengting Yang
Shenzhen University,
China

Should aromatic DBPs be managed as a priority?

MENGTING YANG, SHENZHEN UNIVERSITY, CHINA

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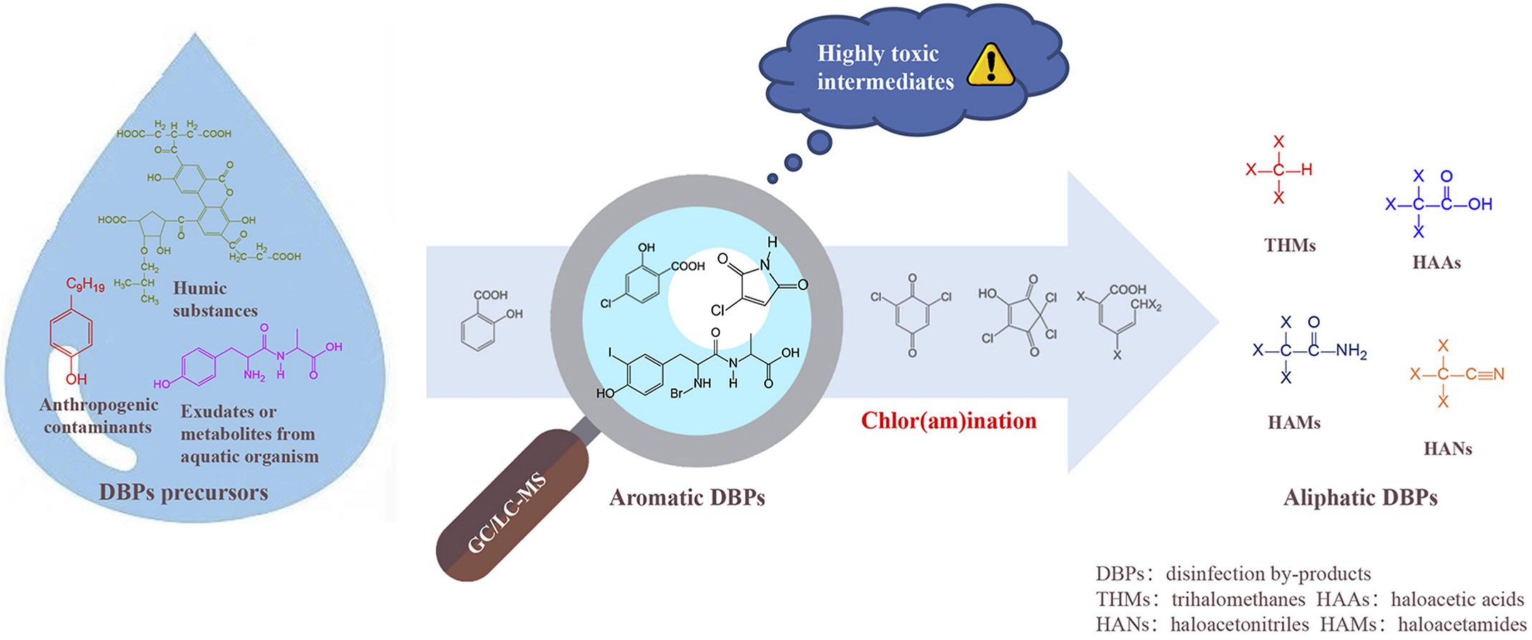
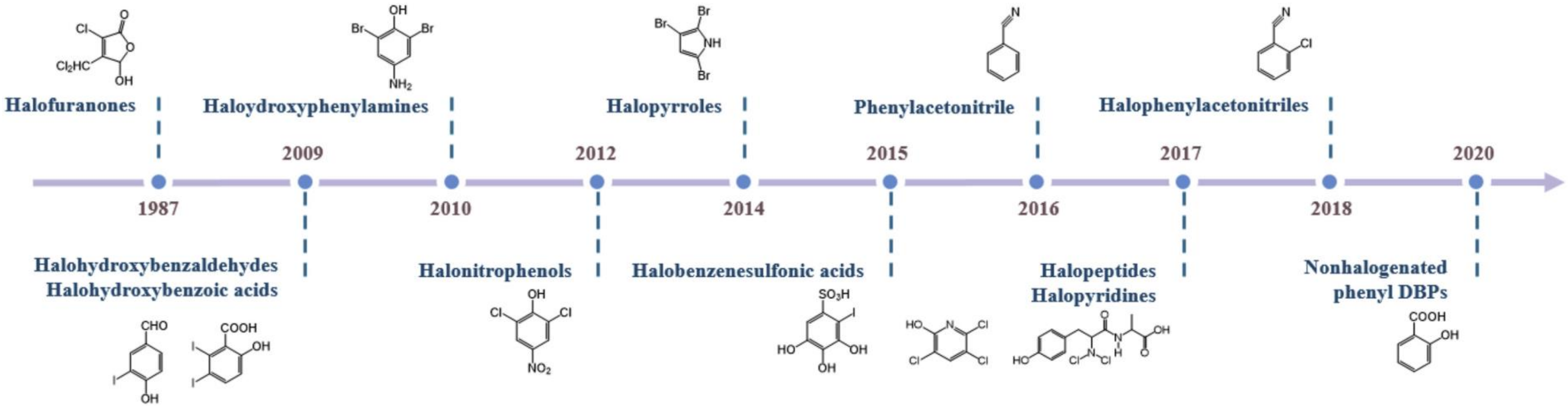
ABOUT THE SPEAKER

- Mengting Yang has been investigating DBPs since 2008.
- She has been responsible for 9 projects including 2 National Natural Science Foundation of China projects, and has published 24 articles (including 6 *ES&T* articles and *4* WR articles) as the first author or corresponding author.
- She won the 2022 ES&T Excellence in Review Award.

AROMATAIC DBPS

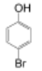
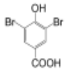
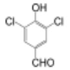
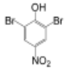
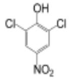
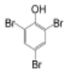
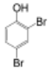
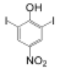
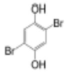
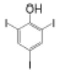
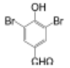


(Liu et al., Water Res., 2020, 116076)



IDENTIFICATION AND OCCURRENCE OF AROMATIC DBPS

- Identified and detected in drinking water and sewage effluent

m/z (RT, min)	Structure	Occurrence[a]	*m/z* (RT, min)	Structure	Occurrence[a]
171/173 (6.06)[b]		a,b,c	293/295/297 (3.55)		a
189/191/193 (4.29)[b]		a,b,c	294/296/298 (6.55)		a,b,c
206/208/210 (4.57)[b]		a,b,c	327/329/331/333 (8.03)		a,b,c
249/251/253 (7.25)[b]		a,b,c	390 (6.60)[b]		a
265/267/269 (4.99)[b]		a,b	471 (8.47)[b]		a
277/279/281 (4.67)		a,b,c			

Yang and Zhang, ES&T, 2013

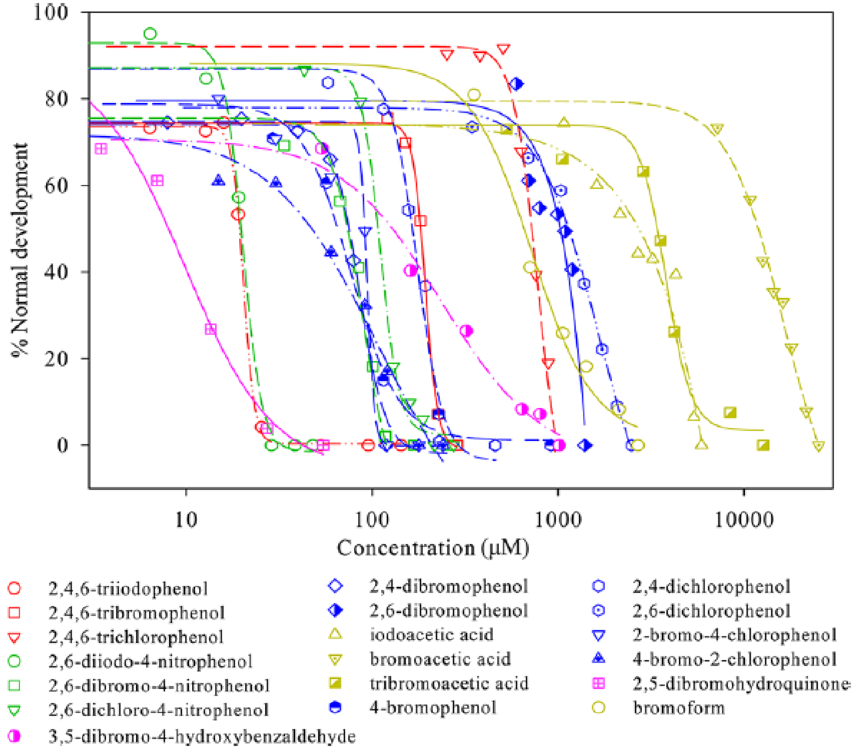
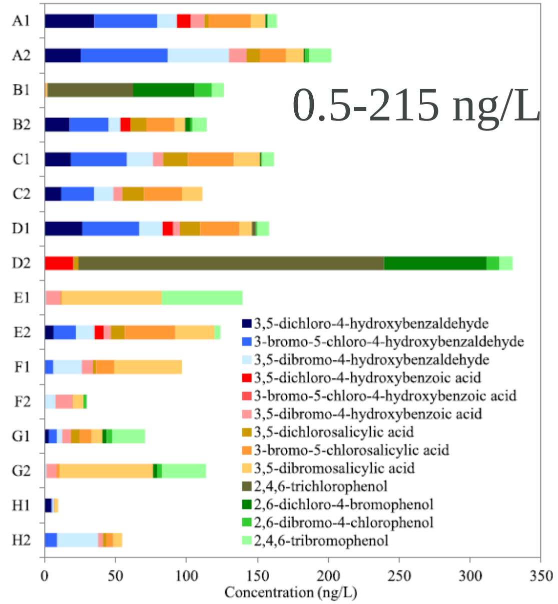
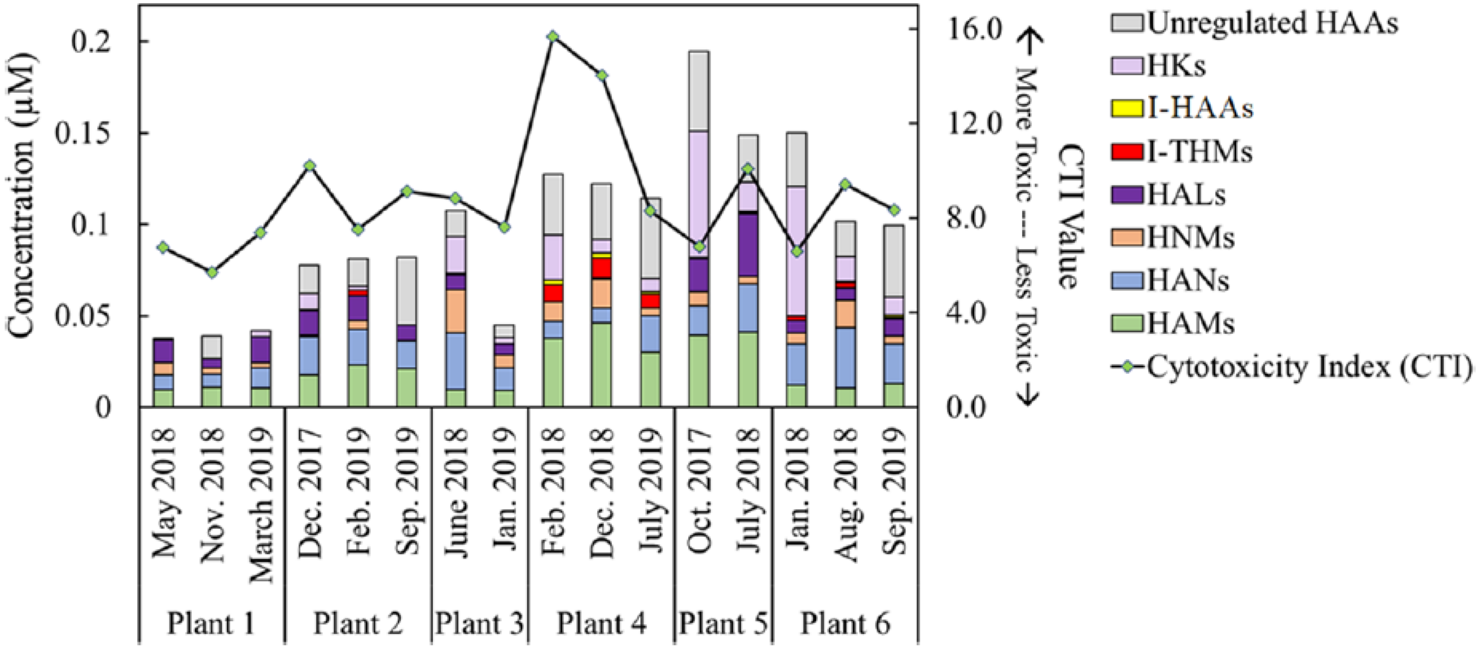


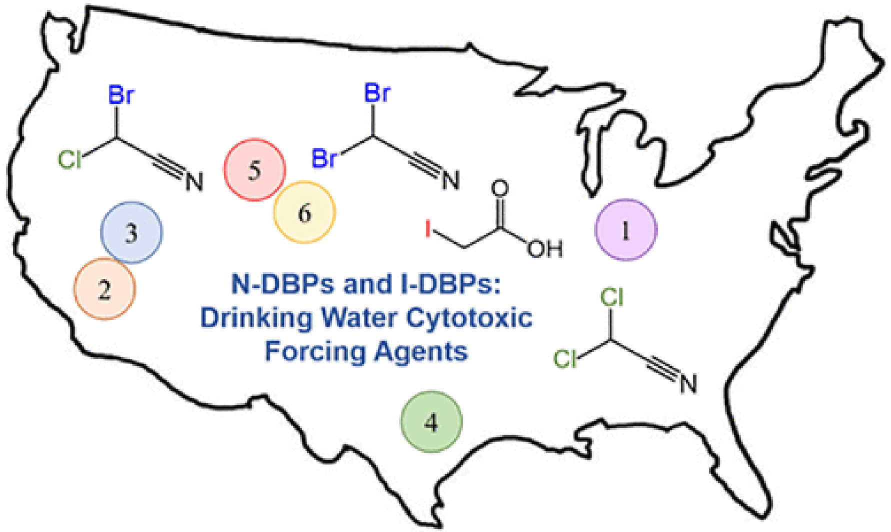
Figure 1. Concentration−response curves of the developmental toxicity of 19 DBPs to *P. dumerilii* embryos.



Pan, et al., Water Res., 2017

- Key DBP toxicity drivers in drinking water across the United States





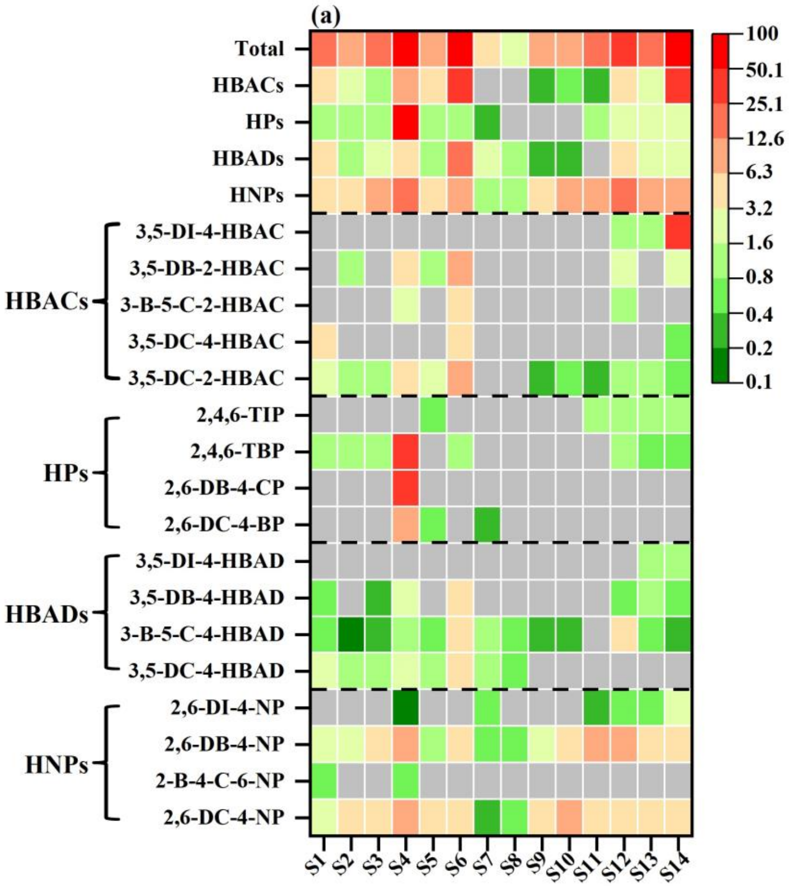
(Allen et al., *Environ. Sci. Technol.*, 2022, 56, 392–402)

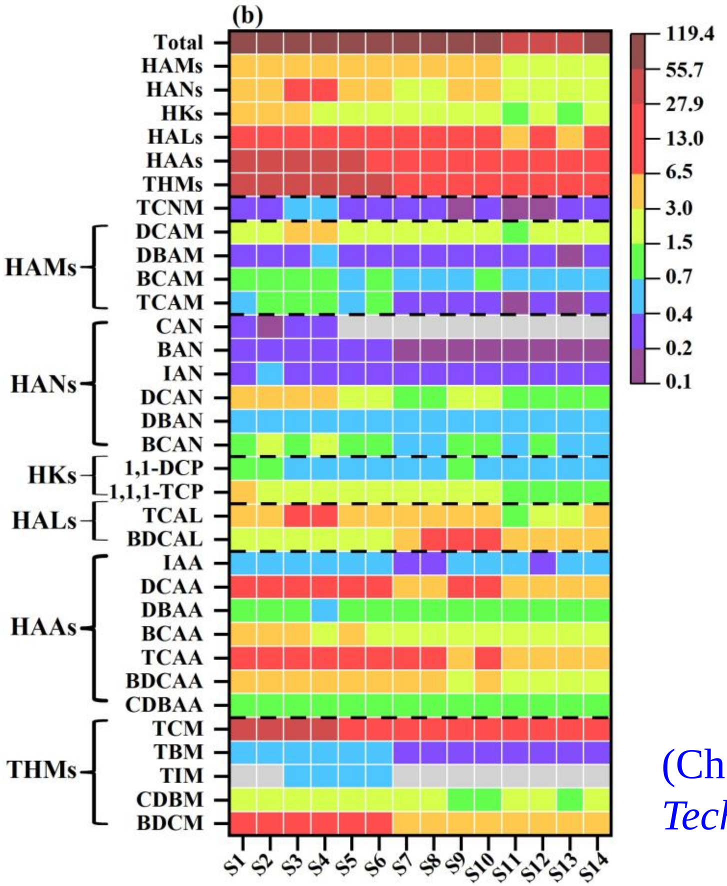
OCCURRENCE OF AROMATIC AND ALIPHATIC HALOGENATED DBPS

- Chlorinated drinking water samples were collected from six DWTPs or their distribution systems in the megacity Shenzhen.
- 11 categories of 56 halogenated DBPs were measured.

Aromatic DBPs
(2+17)

Total concentrations: 1.9−99.9 ng/L





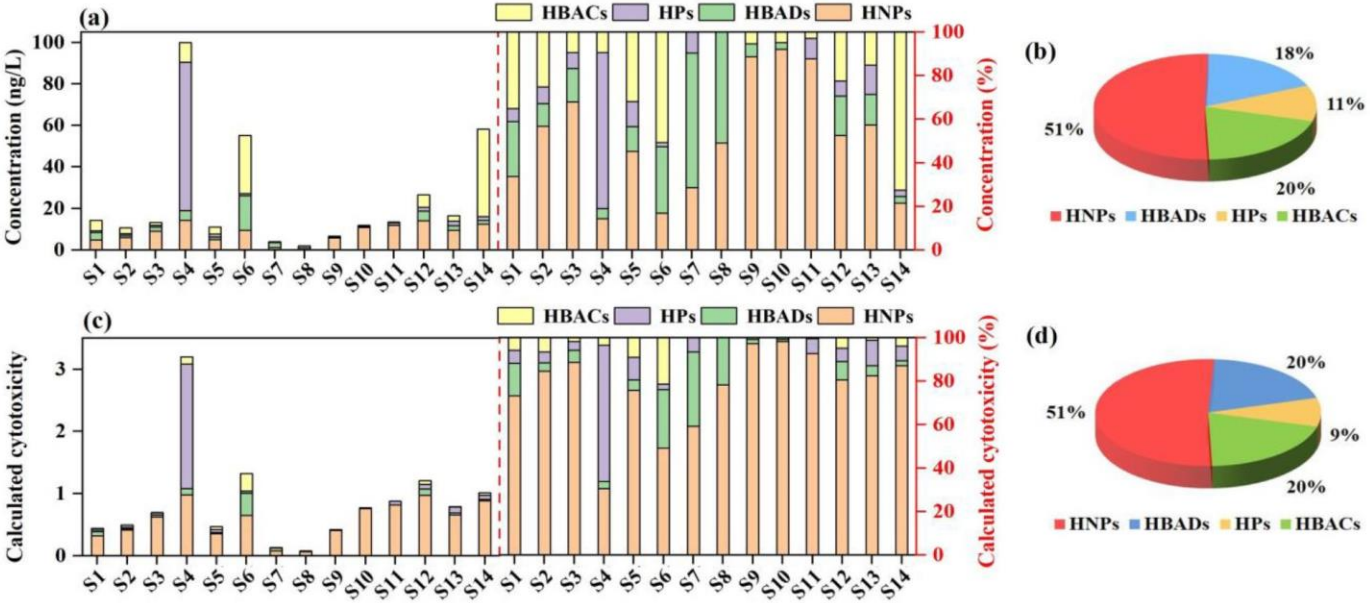
Aliphatic DBPs
(10+27)

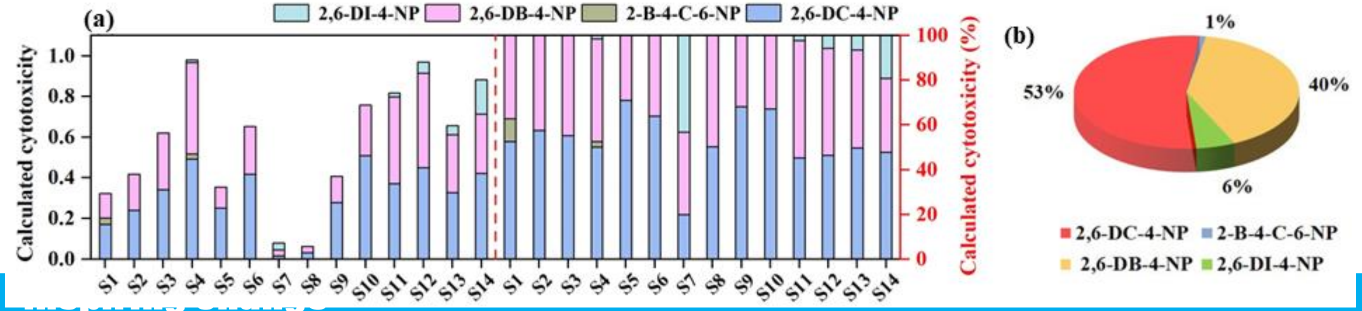
Total concentrations: 35.9−112.3 μg/L

(Chen et al., *Environ. Sci. Technol., 2023*, 57, 1366–1377.)

EVALUATION OF CALCULATED TOXICITY FORCING AGENTS

- **HNPs** play an important role in both total concentration and total calculated cytotoxicity of aromatic DBPs.





Concentration percentage:

HNPs > HBACs > HBADs > HPs

Total calculated drinking water toxicity $= \Sigma\ (C_{DBP} \times LC_{50}^{-1} \times 10^{6})$

Concentration-cytotoxicity percentage:

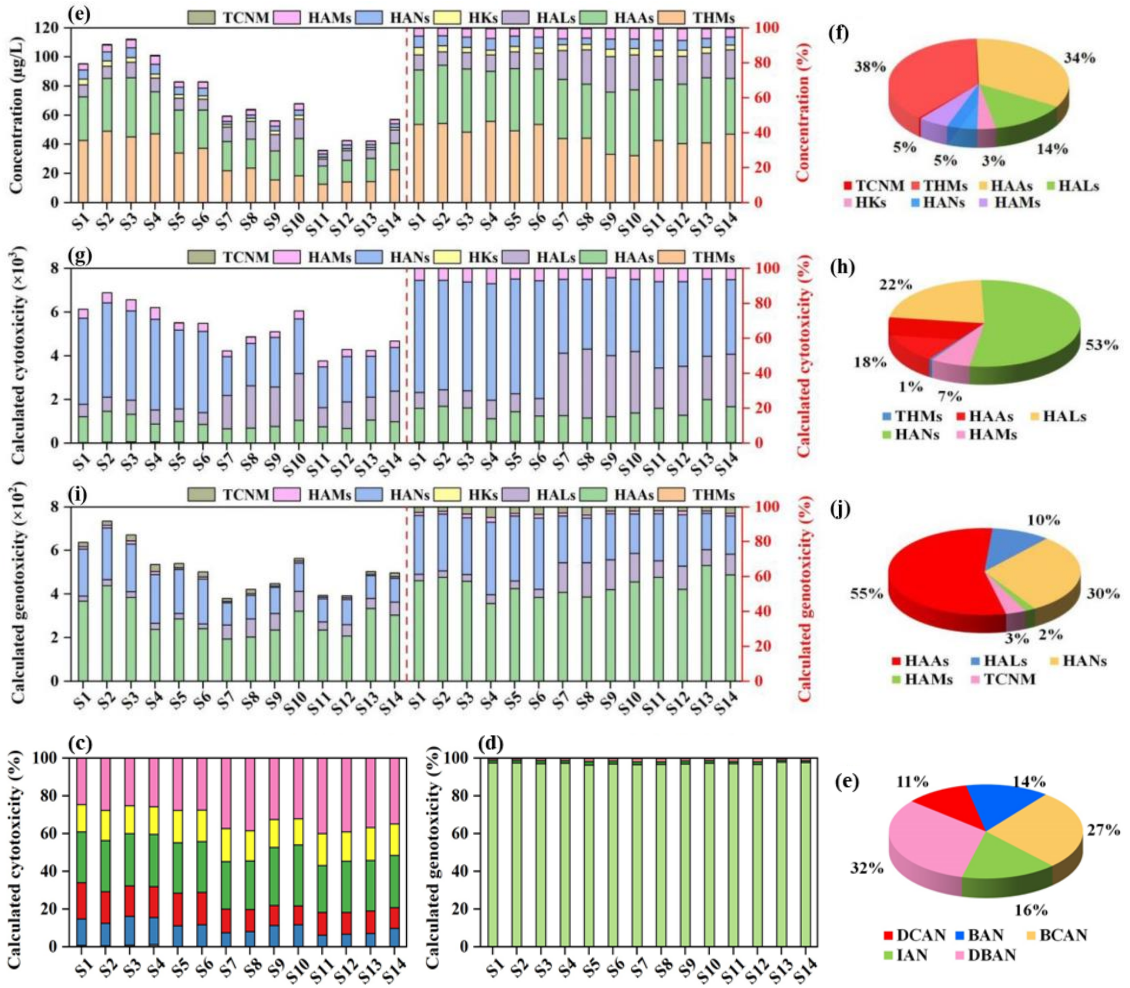
HNPs > HBADs ≈ HBACs > HPs

Calculated toxicity forcing agents:

2,6-DC-4-NP > 2,6-DB-4-NP > 2,6-DI-4-NP > 2-B-4-C-6-NP

EVALUATION OF CALCULATED TOXICITY FORCING AGENTS

- Toxicity drivers identified differ with various toxicity



Concentration percentage :

THMs > HAAs > HALs > HANs ≈ HAMs > HKs > TCNM

Concentration-cytotoxicity percentage :

HANs > HALs > HAAs > HAMs > THMs

Concentration-genotoxicity percentage :

HAAs > HANs > HALs > TCNM > HAMs

Calculated cytotoxicity forcing agents :

DBAN > BCAN > IAN > BAN > DCAN

Calculated genotoxicity forcing agents :

IAA

EVALUATION OF CALCULATED TOXICITY FORCING AGENTS

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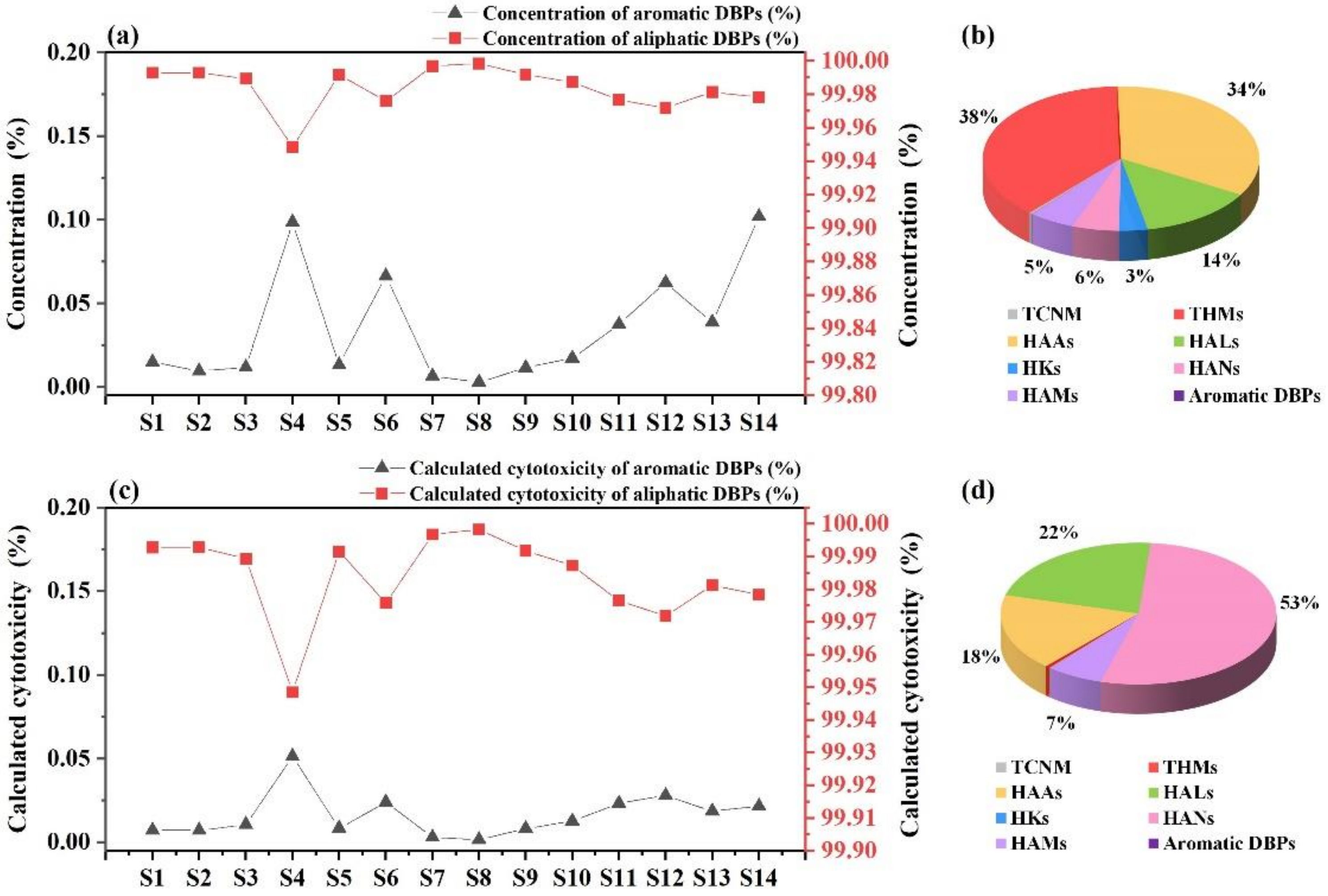
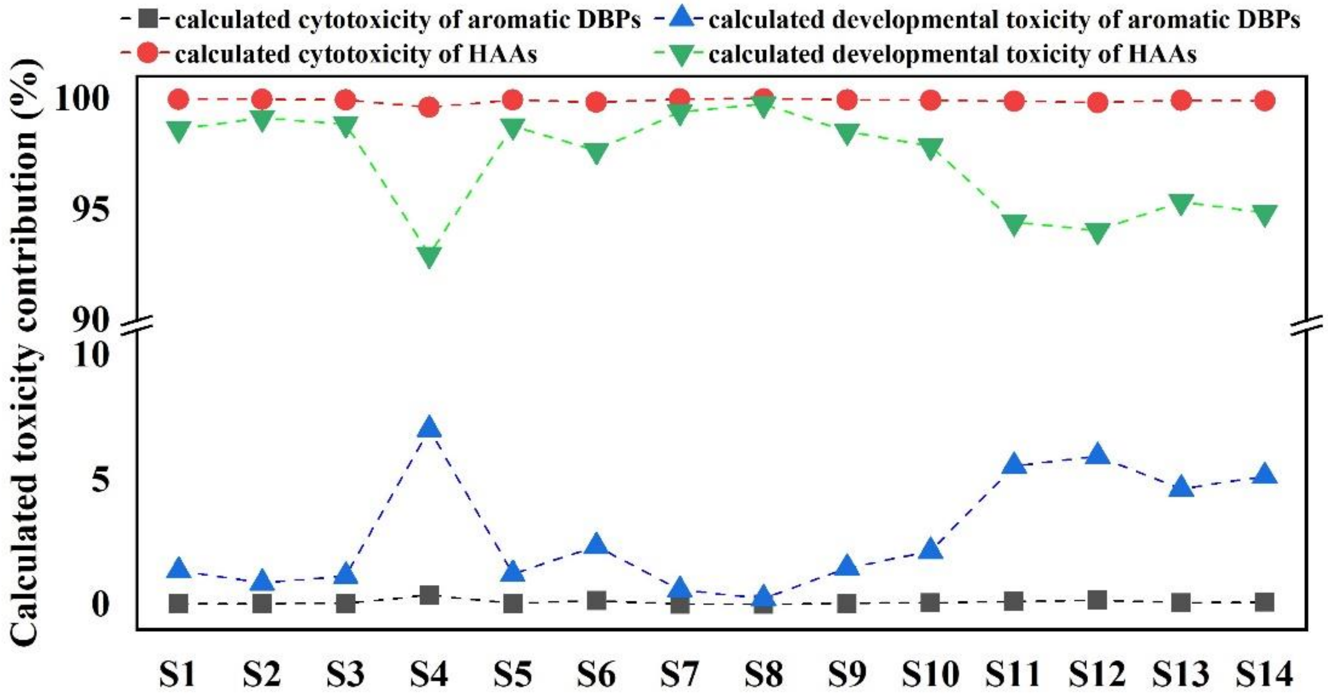
- Key large group of DBPs ?
- Aliphatic species OR

aromatic DBPs ？



COMPARISON OF CALCULATED TOXICITY CONTRIBUTIONS

- Aromatic DBPs vs HAAs



Concentration-toxicity percentages of the **aromatic DBPs**:

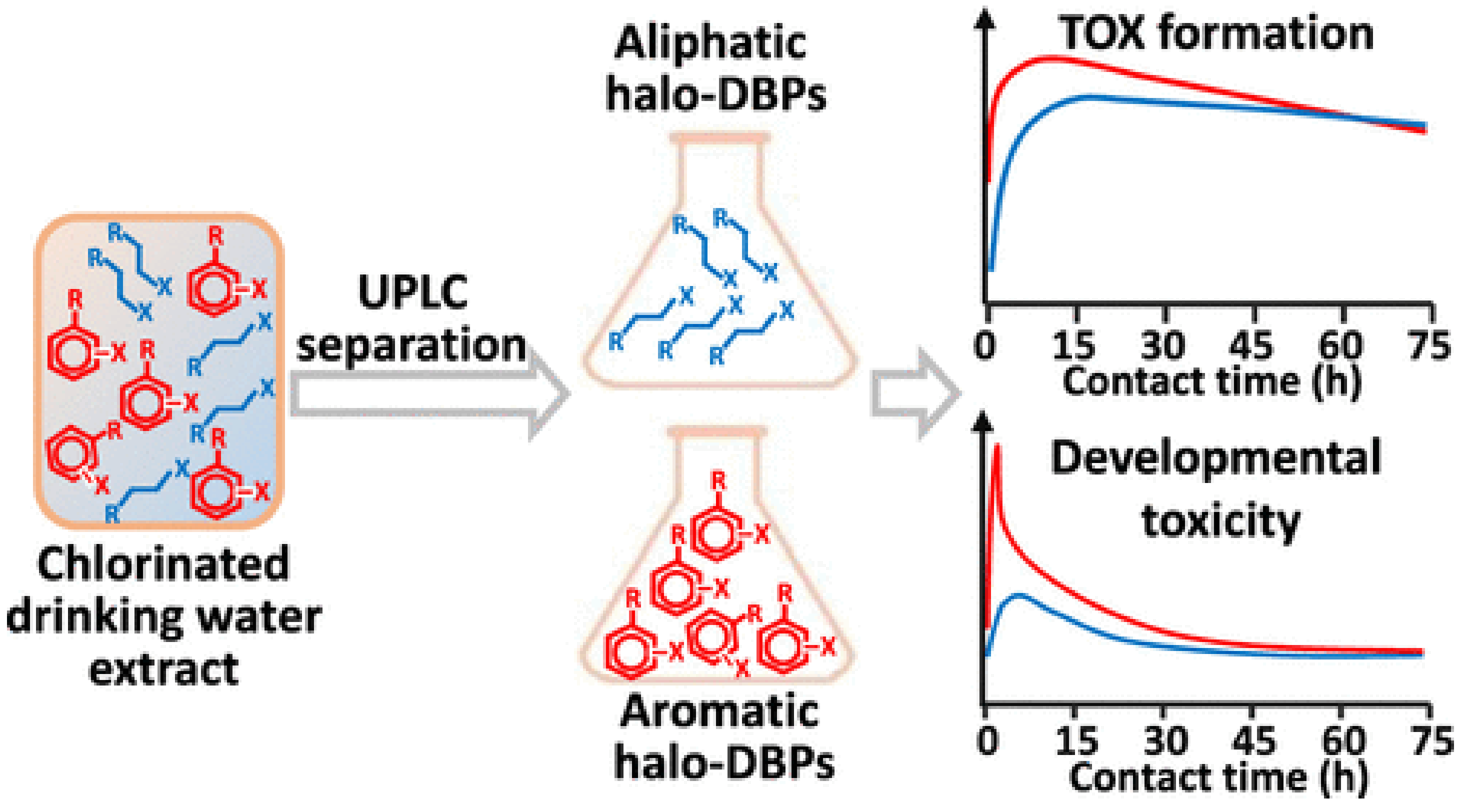
Cytotoxicity endpoint: **< 0.2%**

Developmental toxicity endpoint: **0.2–7.0%**

Developmental toxicity potentials were predicted according to our published QSAR model (*Environ. Sci. Technol.* 2013, 47, 10868–10876):

$$\log EC_{50}^{-1} = 0.3535\log P + 0.7243pK_a - 1.7101E_{LUMO} - 1.4132E_{HOMO} - 22.5945$$

AROMATIC DBPS VS ALIPHATIC DBPS



TOX concentration:
aromatic fractions > aliphatic fractions

Developmental toxicity:
aromatic fractions > aliphatic fractions

(Han et al., *Environ. Sci. Technol.*, 2021, 55, 5906–5916)

STATISTICAL ANALYSES

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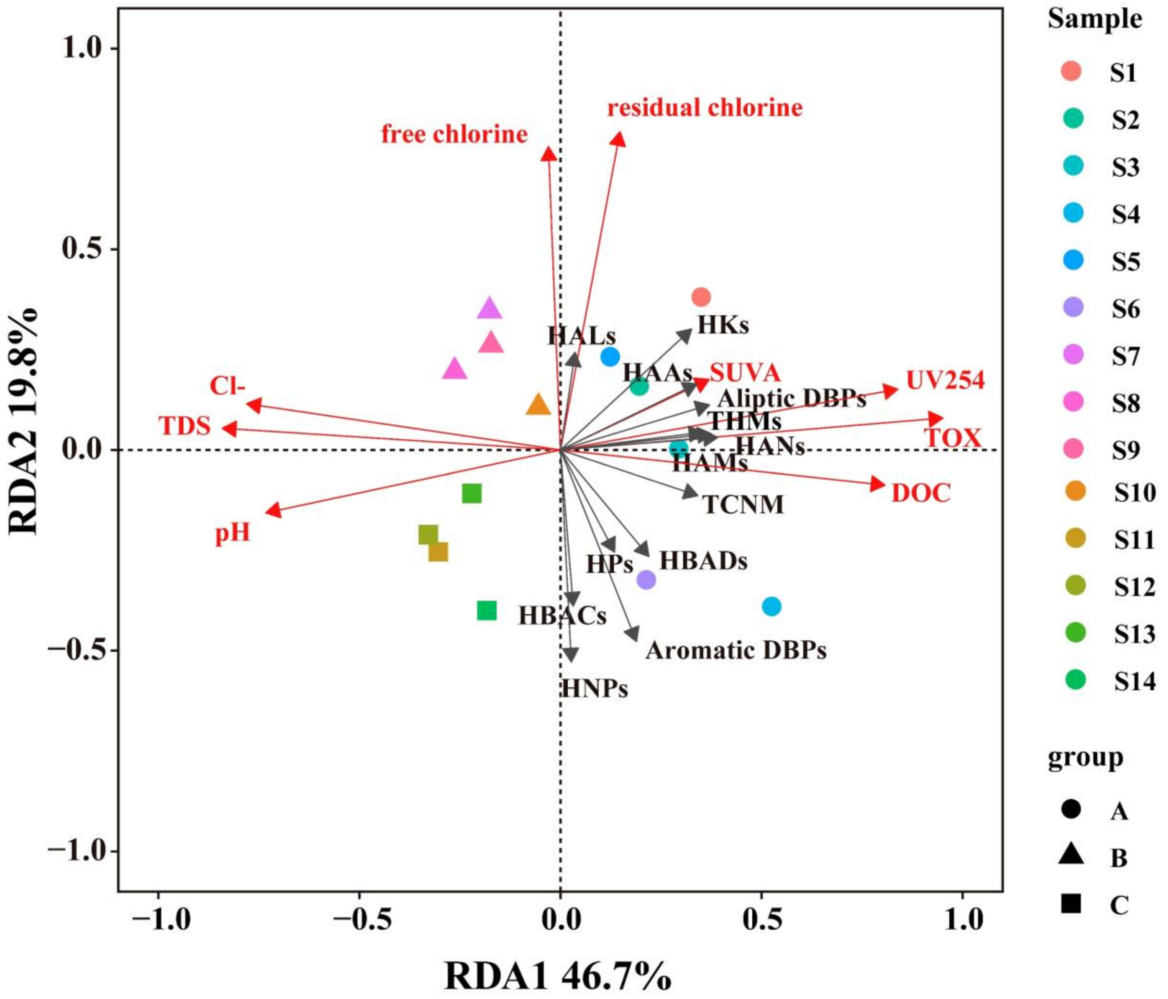
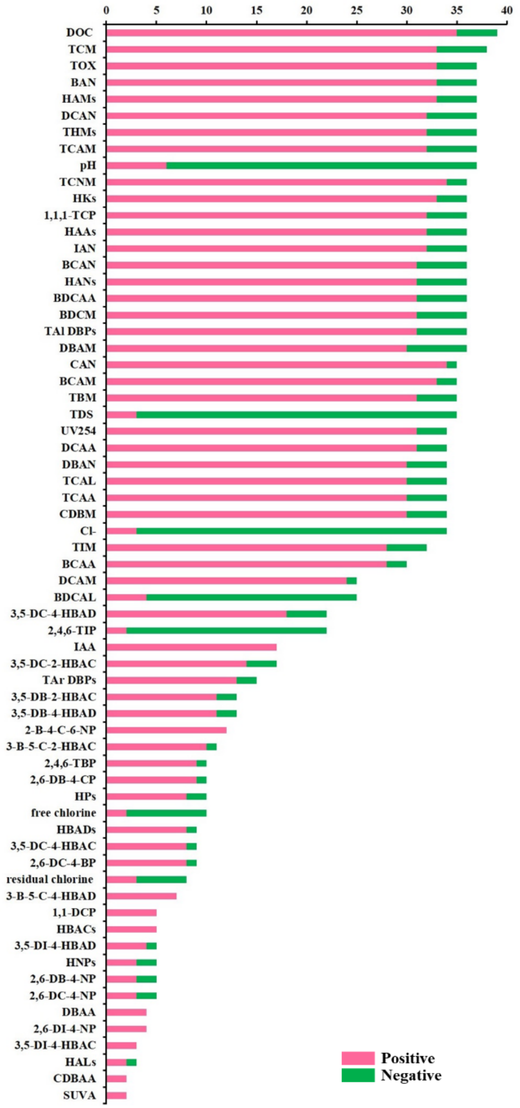


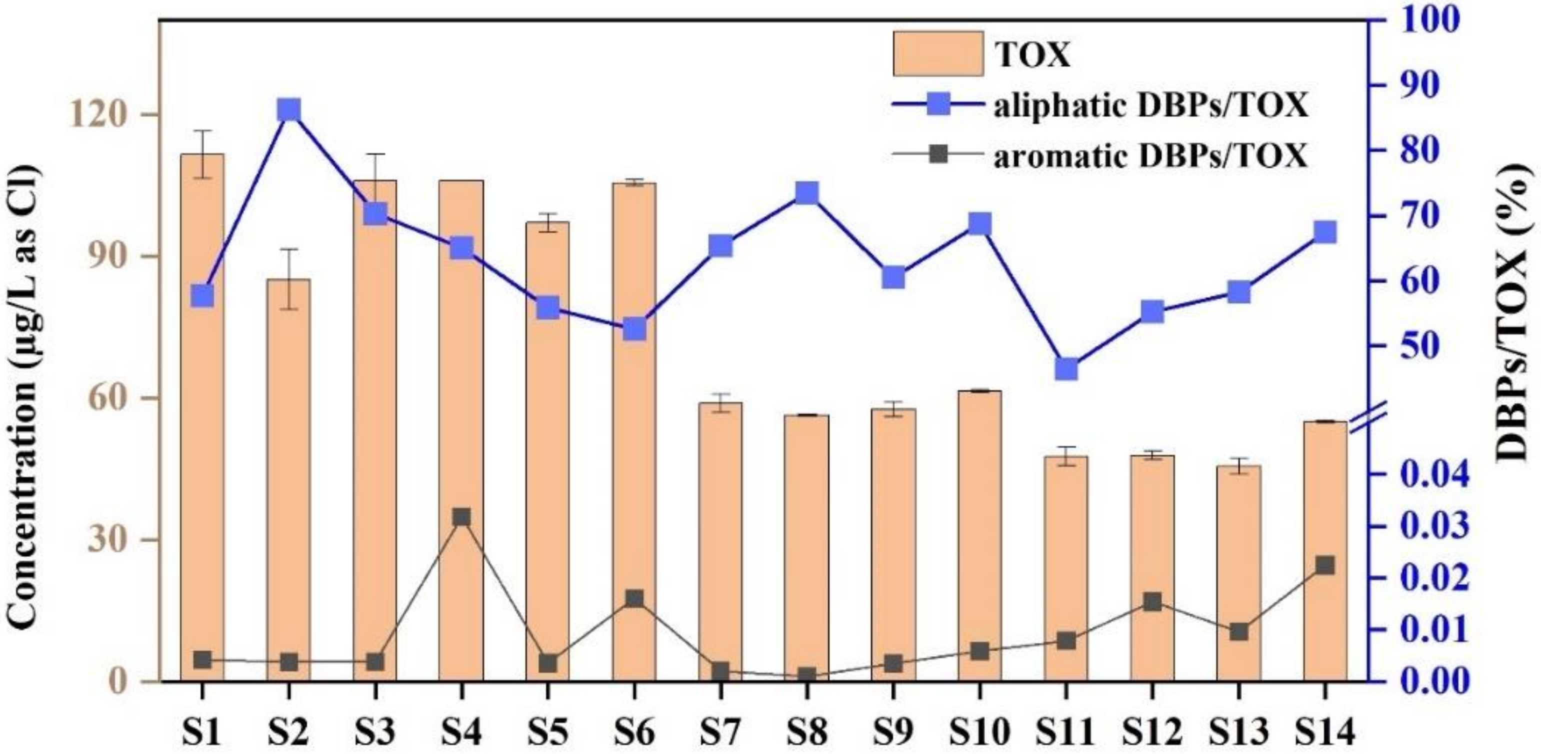


- The water quality were affected by geographic location and the way of water treatment.
- TOX showed significant positive correlations with most aliphatic DBPs but no aromatic DBPs.
- DOC and UV_{254} were important parameters to predict DBP formation.

TOX CONCENTRATIONS

- Extremely low contribution of the measured aromatic DBPs may be the reason for no correlation between TOX and aromatic DBPs.
- A more comprehensive and representative set of aromatic DBPs should be further explored.

  - Total concentrations of measured aromatic DBPs: 1.9−99.9 ng/L (<1.0% of the TOX)
  - Total concentrations of measured aliphatic DBPs: 35.9−112.3 μg/L (46.5−86.3% of the TOX)



CORRELATIONS BETWEEN OVERALL CYTOTOXICITY AND DBP FORMATION

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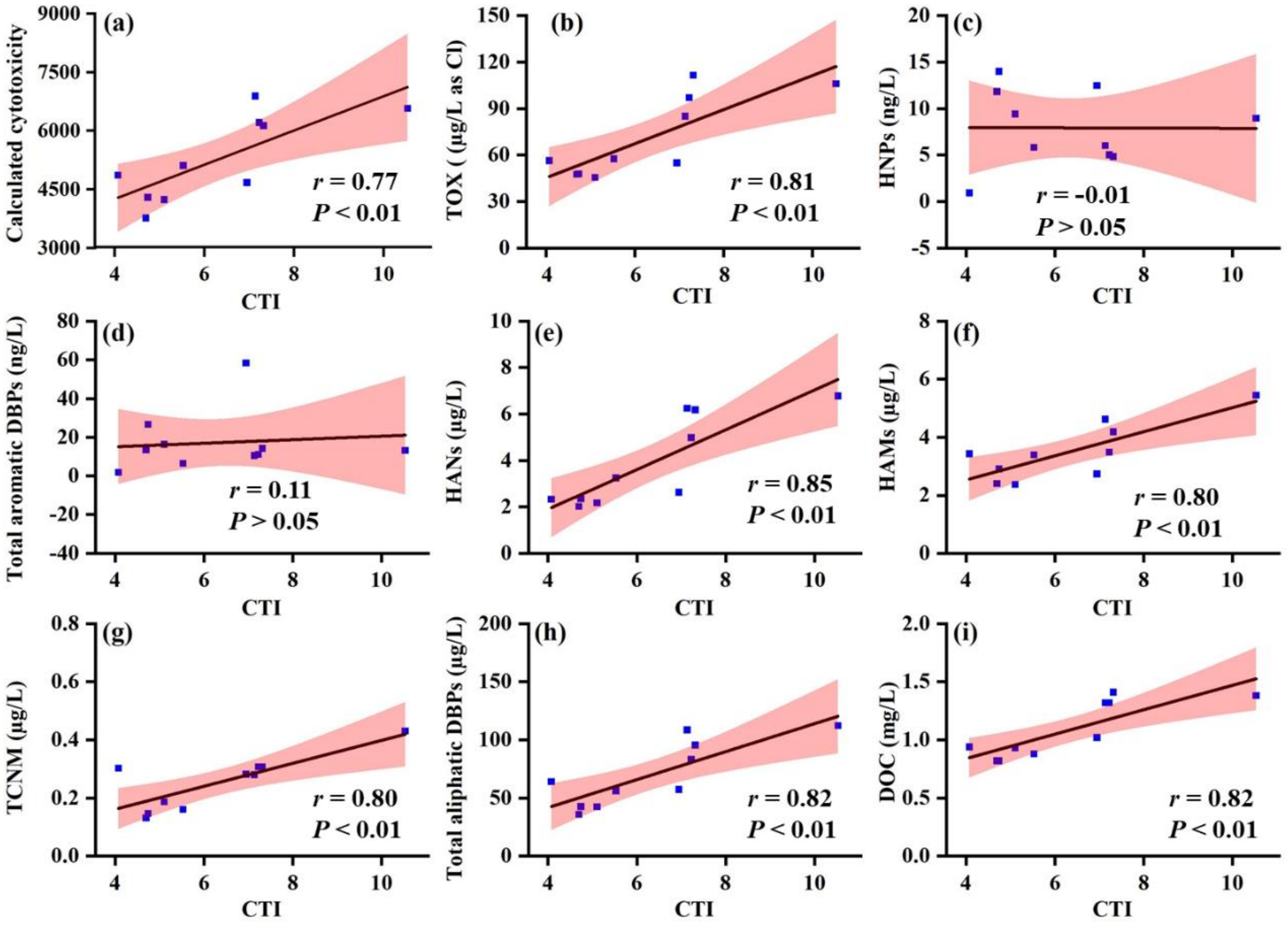
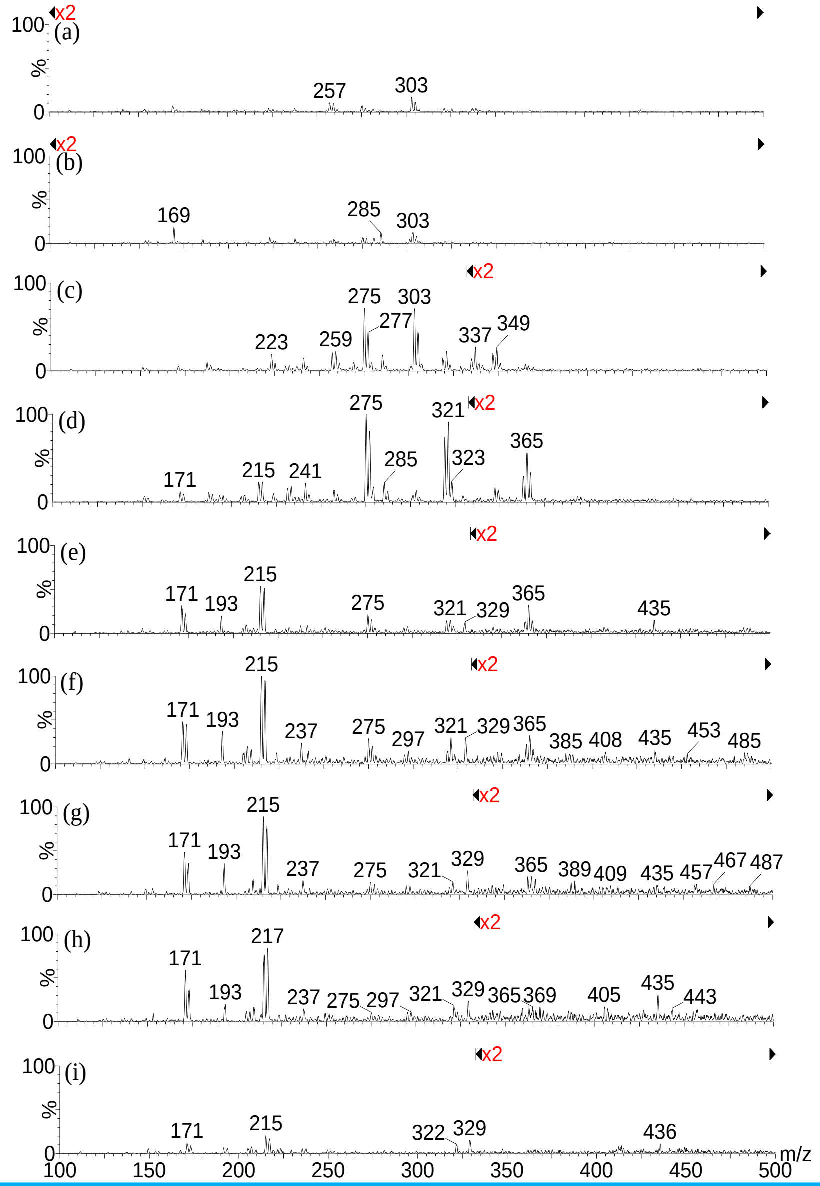
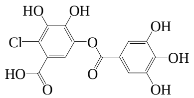
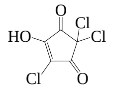
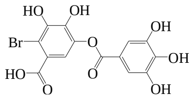
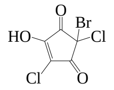
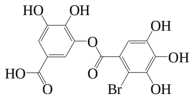
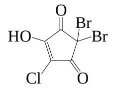
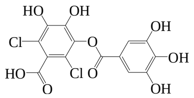
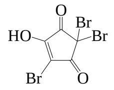
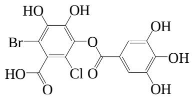
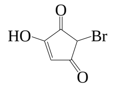
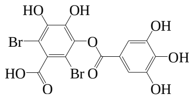
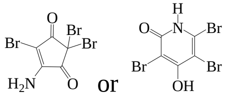
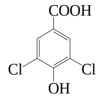
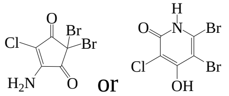
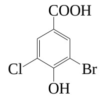
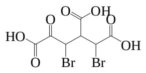
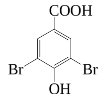
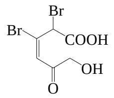
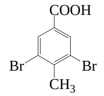
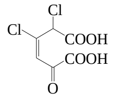
- The overall cytotoxicity of drinking water — assessed with in vitro CHO cell cytotoxicity assay
- CTI vs total calculated cytotoxicity
- Total concentration of aliphatic DBPs, three classes of N-DBPs
- DOC and TOX are important overall cytotoxicity indicators

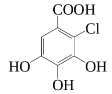
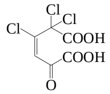
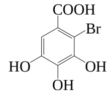
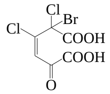
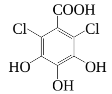
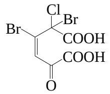
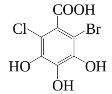
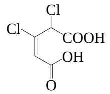
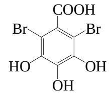
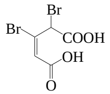
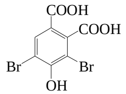
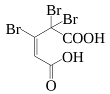
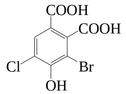
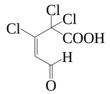
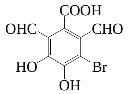
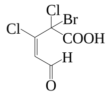
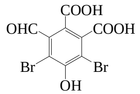
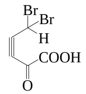
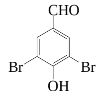
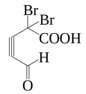
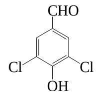
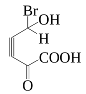


NEW DBPS DERIVED FROM TANNIC ACID AND ITS BIODEGRADATION PRODUCTS

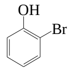
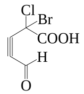
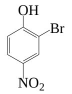
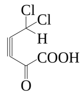
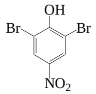
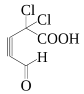
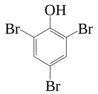
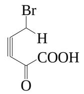
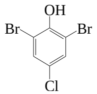
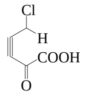
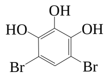
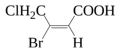
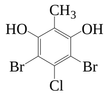
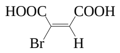
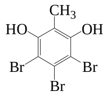
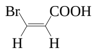
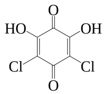
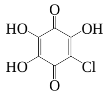
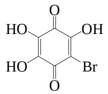


Code (Ratio)	*m/z* (Formula)	Proposed structure	Δ[a] (ppm)	Code (Ratio)	*m/z* (Formula)	Proposed structure	Δ[a] (ppm)
A-I (3:1)	355/357[c] $C_{14}H_9O_9Cl$		1.83	D-I (27:27:9:1)	213/215/217/219 $C_5HO_3Cl_3$		5.56
A-II (1:1)	399/401[c] $C_{14}H_9O_9Br$		0.12	D-II (9:15:7:1)	257/259/261/263 $C_5HO_3BrCl_2$		2.31
A-III (1:1)	399/401[c] $C_{14}H_9O_9Br$		0.63	D-III (3:7:5:1)	301/303/305/307 $C_5HO_3Br_2Cl$		9.87
A-IV (9:6:1)	389/391/393[c] $C_{14}H_8O_9Cl_2$		0.42	D-IV (1:3:3:1)	345/347/349/351 $C_5HO_3Br_3$		3.46
A-V (3:4:1)	433/435/437[c] $C_{14}H_8O_9BrCl$		0.38	D-V (1:1)	189/191[c] $C_5H_3O_3Br$		2.89
A-VI (1:2:1)	477/479/481[c] $C_{14}H_8O_9Br_2$		1.18	D-VI (1:3:3:1)	344/346/348/350[c] $C_5H_2O_2Br_3N$		1.37
B-I (9:6:1)	205/207/209 $C_7H_4O_3Cl_2$		5.96	D-VII (3:7:5:1)	300/302/304/306[b, c] $C_5H_2O_2Br_2ClN$		/
B-II (3:4:1)	249/251/253 $C_7H_4O_3BrCl$		5.44	E-I (1:2:1)	359/361/363[b, c] $C_7H_6O_7Br_2$		/
B-III (1:2:1)	293/295/297 $C_7H_4O_3Br_2$		9.50	E-II (1:2:1)	299/301/303[c] $C_6H_6O_4Br_2$		9.09
B-IV (1:2:1)	291/293/295[c] $C_8H_6O_2Br_2$		4.78	E-III (9:6:1)	225/227/229[c] $C_6H_4O_5Cl_2$		2.20

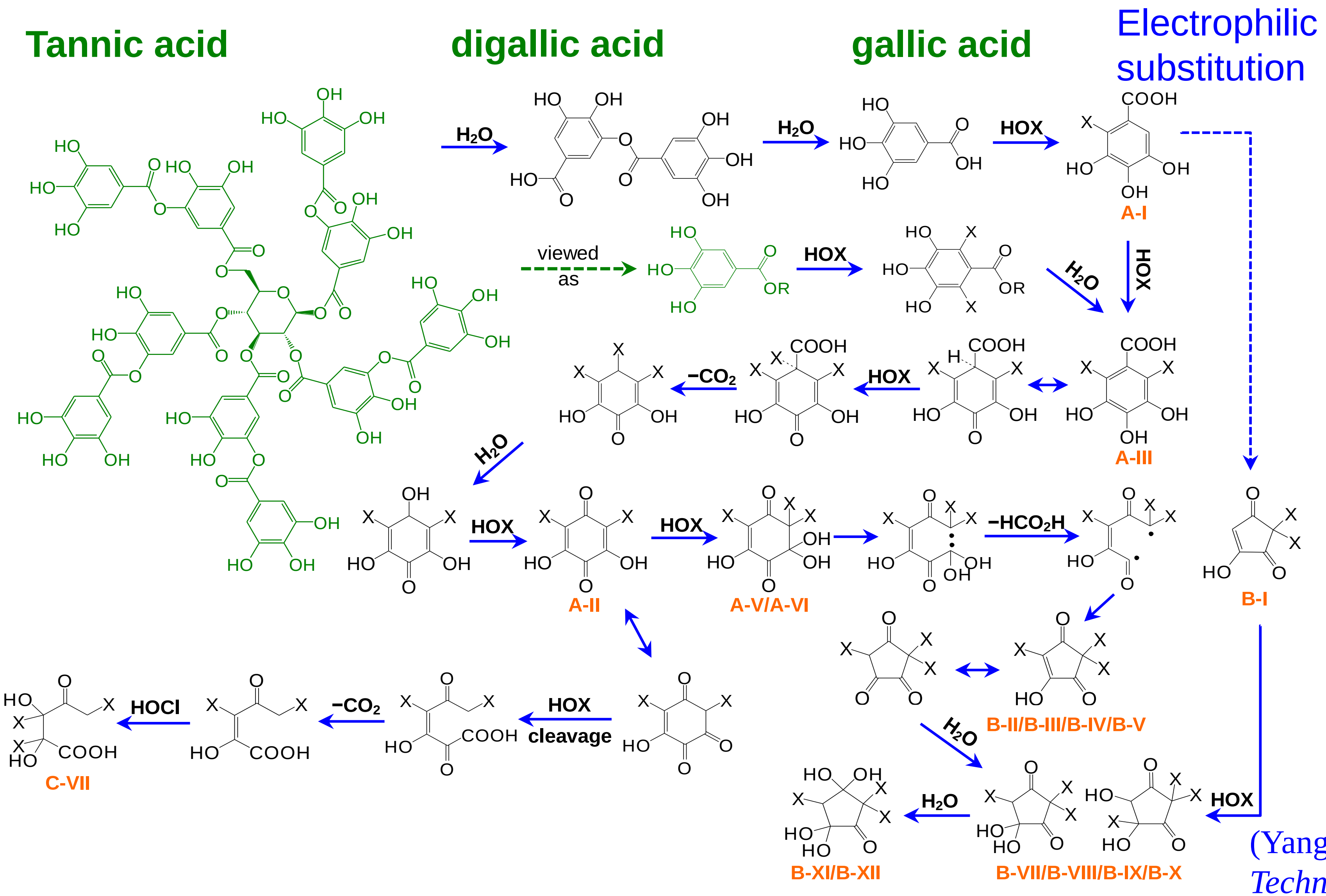
NEW DBPS DERIVED FROM TANNIC ACID AND ITS BIODEGRADATION PRODUCTS

Code (Ratio)	*m/z* (Formula)	Proposed structure	Δ[a] (ppm)	Code (Ratio)	*m/z* (Formula)	Proposed structure	Δ[a] (ppm)
B-V (3:1)	203/205 $C_7H_5O_5Cl$		4.66	E-IV (27:27:9:1)	259/261/263/265 $C_6H_3O_5Cl_3$		3.90
B-VI (1:1)	247/249[c] $C_7H_5O_5Br$		4.03	E-V (9:15:7:1)	303/305/307/309 $C_6H_3O_5BrCl_2$		8.25
B-VII (9:6:1)	237/239/241 $C_7H_4O_5Cl_2$		1.54	E-VI (3:7:5:1)	347/349/351/353[c] $C_6H_3O_5Br_2Cl$		1.08
B-VIII (3:4:1)	281/283/285[c] $C_7H_4O_5BrCl$		6.48	E-VII (9:6:1)	197/199/201[c] $C_5H_4O_4Cl_2$		4.35
B-IX (1:2:1)	325/327/329[c] $C_7H_4O_5Br_2$		6.94	E-VIII (1:2:1)	285/287/289[c] $C_5H_4O_4Br_2$		4.99
B-X (1:2:1)	337/339/341[c] $C_8H_4O_5Br_2$		3.74	E-IX (1:3:3:1)	363/365/367/369[c] $C_5H_3O_4Br_3$		0.41
B-XI (3:4:1)	293/295/297[c] $C_8H_4O_5BrCl$		7.80	E-X (27:27:9:1)	215/217/219/221[c] $C_5H_3O_3Cl_3$		2.99
B-XII (1:1)	287/289[c] $C_9H_5O_6Br$		6.42	E-XI (9:15:7:1)	259/261/263/265[c] $C_5H_3O_3BrCl_2$		3.06
B-XIII (1:2:1)	365/367/369[c] $C_9H_4O_6Br_2$		1.54	E-XII (1:2:1)	267/269/271[c] $C_5H_2O_3Br_2$		3.72
B-XIV (1:2:1)	277/279/281 $C_7H_4O_2Br_2$		4.23	E-XIII (1:2:1)	267/269/271[c] $C_5H_2O_3Br_2$		3.72
B-XV (9:6:1)	189/191/193 $C_7H_4O_2Cl_2$		4.83	E-XIV (1:1)	205/207[c] $C_5H_3O_4Br$		3.89

NEW DBPS DERIVED FROM TANNIC ACID AND ITS BIODEGRADATION PRODUCTS

Code (Ratio)	*m/z* (Formula)	Proposed structure	Δ[a] (ppm)	Code (Ratio)	*m/z* (Formula)	Proposed structure	Δ[a] (ppm)
C-I (1:1)	171/173 C_6H_5OBr		1.74	E-XV (3:4:1)	223/225/227[c] $C_5H_2O_3BrCl$		5.64
C-II (1:1)	216/218 $C_6H_4O_3BrN$		1.39	E-XVI (9:6:1)	179/181/183[c] $C_5H_2O_3Cl_2$		3.57
C-III (1:2:1)	294/296/298 $C_6H_3O_3Br_2N$		5.75	E-XVII (9:6:1)	179/181/183[c] $C_5H_2O_3Cl_2$		3.88
C-IV (1:3:3:1)	327/329/331/333 $C_6H_3OBr_3$		1.75	E-XVIII (1:1)	189/191[c] $C_5H_3O_3Br$		2.10
C-V (3:7:5:1)	283/285/287/289[b] $C_6H_3OBr_2Cl$		/	E-XIX (3:1)	145/147[c] $C_5H_3O_3Cl$		3.43
C-VI (1:2:1)	281/283/285[c] $C_6H_4O_3Br_2$		5.07	E-XX (3:4:1)	195/197/199[c] $C_4H_2O_2BrCl$		5.76
C-VII (3:7:5:1)	313/315/317/319[c] $C_7H_5O_2Br_2Cl$		8.48	E-XXI (1:1)	193/195[b, d] $C_4H_3O_4Br$		/
C-VIII (1:3:3:1)	357/359/361/363[c] $C_7H_5O_2Br_3$		1.39	E-XXII (1:1)	149/151[d] $C_3H_3O_2Br$		0.67
C-IX (9:6:1)	207/209/211 $C_6H_2O_4Cl_2$		3.20	E-XXIII (1:2:1)	215/217/219[d] $C_2H_2O_2Br_2$	$CHBr_2COOH$	3.84
C-X (3:1)	189/191[c] $C_6H_3O_5Cl$		4.74	E-XXIV (3:4:1)	171/173/175[d] $C_2H_2O_2BrCl$	CHClBrCOOH	2.89
C-XI (1:1)	233/235[c] $C_6H_3O_5Br$		5.14				

FORMATION MECHANISMS



(Yang et al., *Environ. Sci. Technol.*, *2019*, 53, 13019−13030)

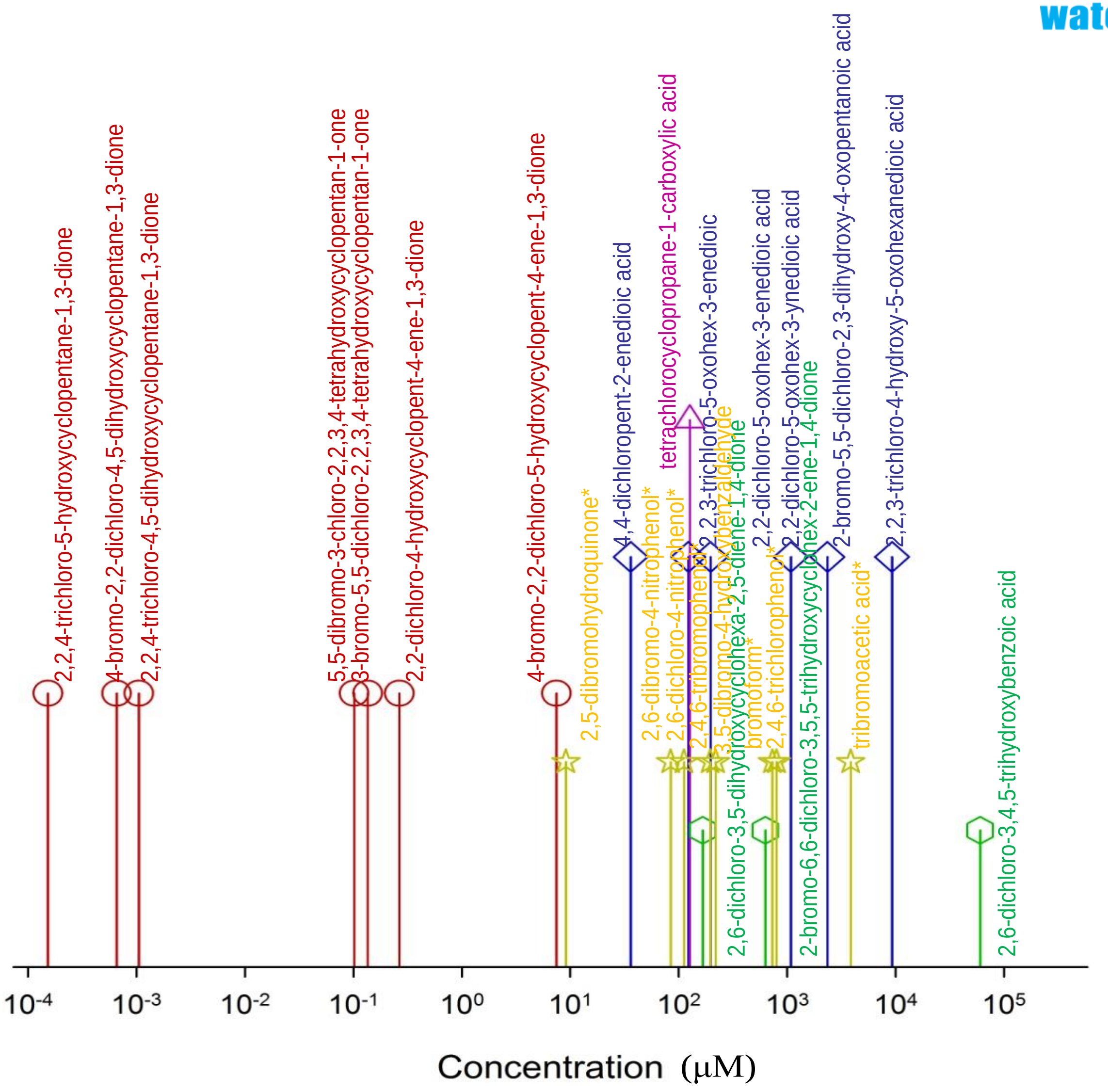
PREDICTED DEVELOPMENTAL TOXICITY

- Emerging DBP group trihalo-(di)hydroxycyclopentane-1,3-diones may possess extremely high toxic potencies.

developmental toxicity to

Platynereis dumerilii:

$$\log EC_{50}^{-1} = 0.3535 \log P + 0.7243\, pKa - 1.7101\, E_{LUMO} - 1.4132\, E_{HOMO} - 22.5945$$



OUTLOOK

- Current reported aromatic DBPs are insufficient to represent the overall aromatic DBPs.
- The composition of TOX remains largely unknown and will be identified successively in the future due to the improvement of analytical techniques.
- Databases of toxicity potencies of individual DBPs and prediction models need further development.
- Combined analyses of calculated toxicity and experimental overall toxicity of real water samples should be conducted in future studies.
- If the calculated toxicity of a given individual aromatic DBP correlates well with the overall toxicity of the aromatic fraction, a suspected toxicity driver for aromatic DBPs can be found.
- Effect-directed analysis would be a useful tool for finding priority DBPs.

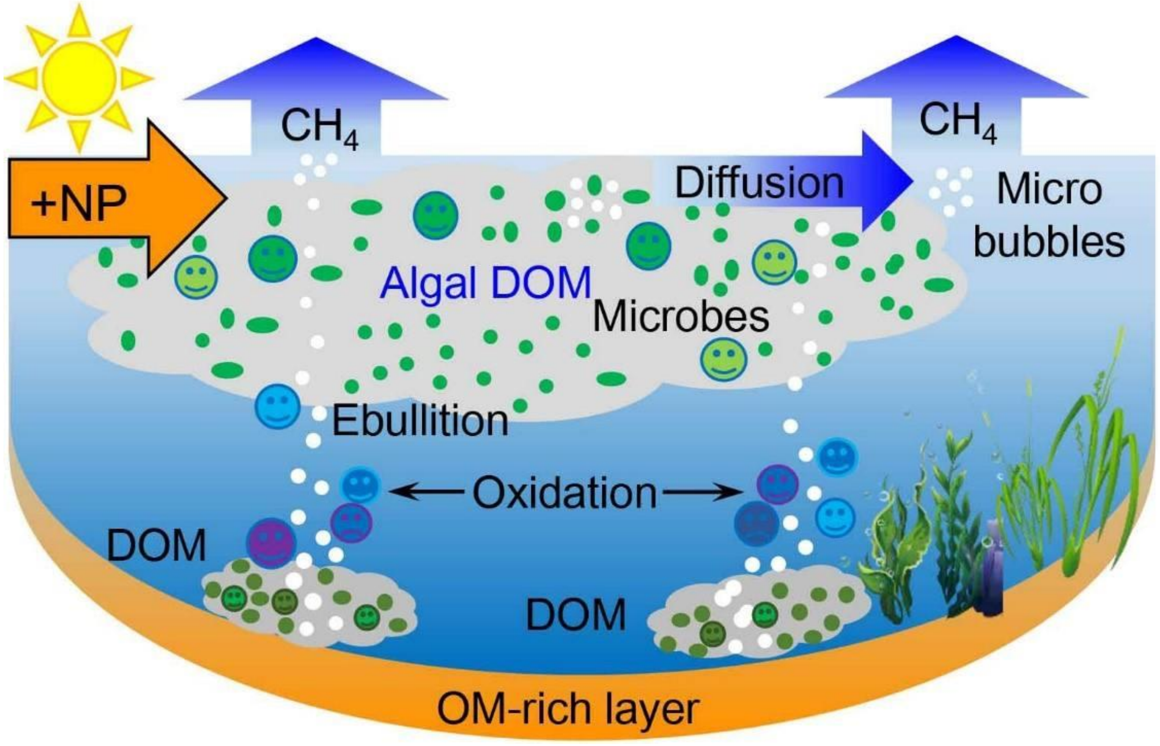
Understanding the Radical Involved Reactions of Dissolved Organic Matter: Kinetics and DBP Formation

Xin Yang

Sun Yat-sen University

24 April, 2024

DOM is ubiquitous in water



Dissolved

Organic

Matter

- Fulvic Acids
- Humic acids
- Phenolics
- Amino acids
- Aliphatic acids
- Hydrocarbons
- ...

Dissolved organic matter (DOM) is a complex mixture.

Chappaz*, Curtis, *Environ. Sci. Technol*. **2013**, 47, 4, 2001–2007

DOM is ubiquitous in water

- **Heterogeneous mixtures**

  dispersed matter and continuum with different physical properties

- **A wide range of molecular weight**

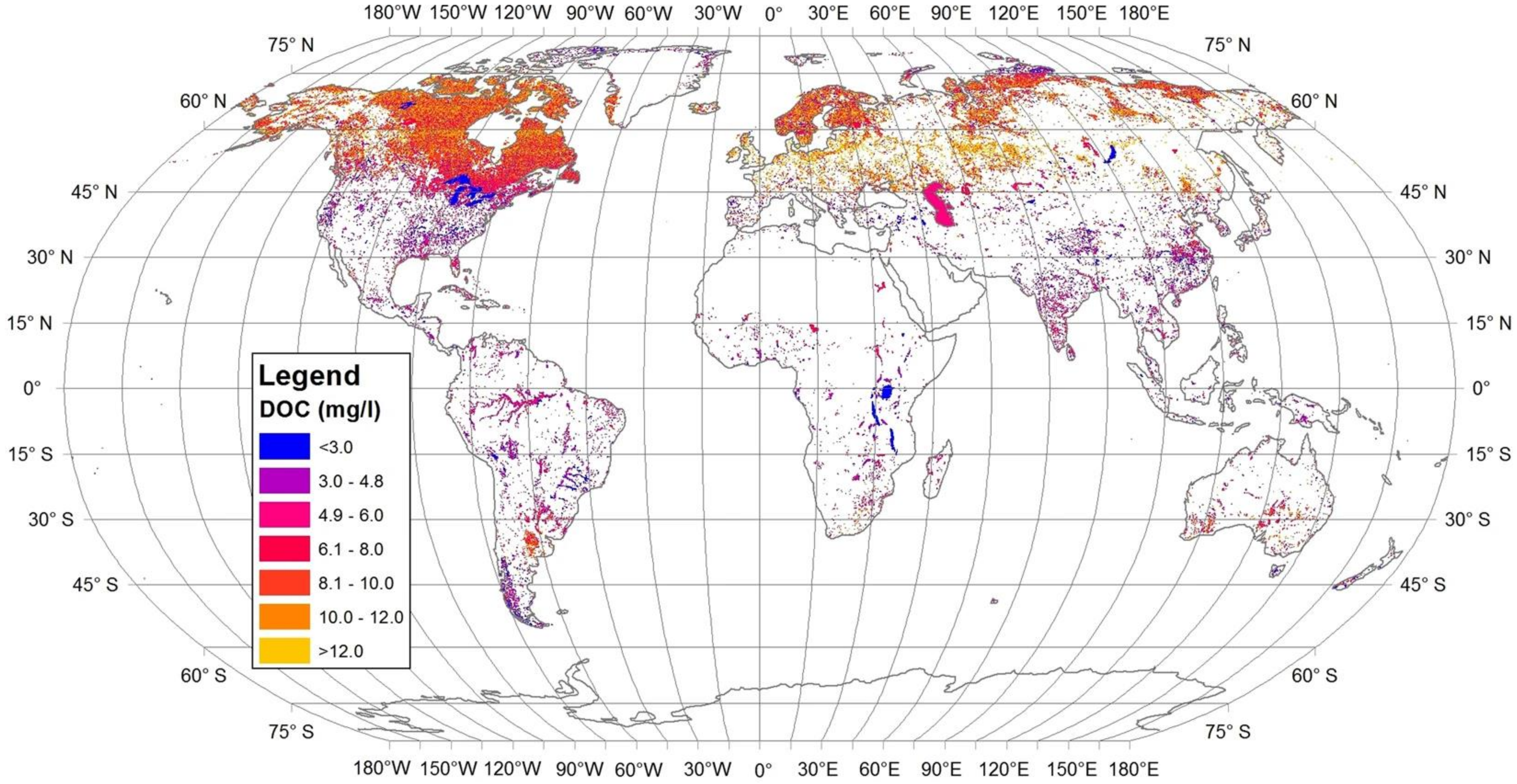
  <500 to >10,000 Dalton

- **Complicated structure**

  Containing diverse moieties and functional groups (–COOH, –OH, –CHO, –COR, –C=OR, –NH_2, etc.)

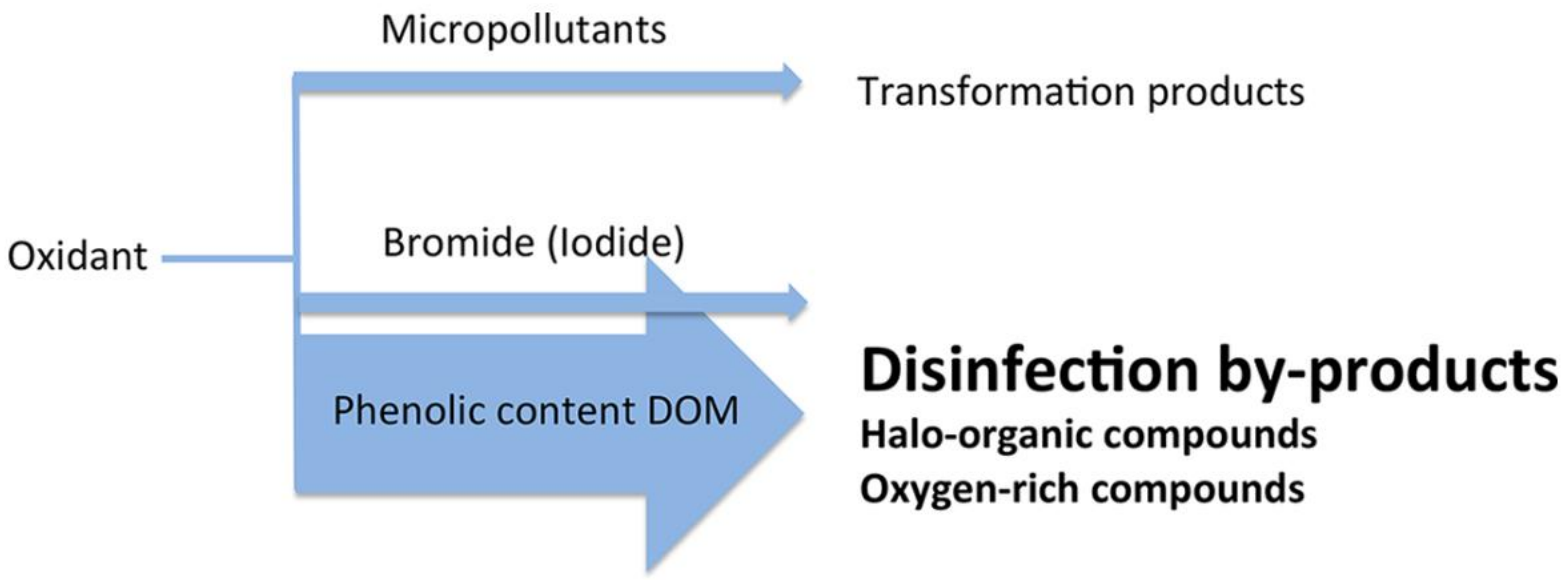
Nature organic matter (NOM), Effluent organic matter (EfOM), Algae organic matter (AOM)

DOM is ubiquitous in water



https://www.nature.com/articles/s41598-020-65010-3

DOM as the precursor of DBPs



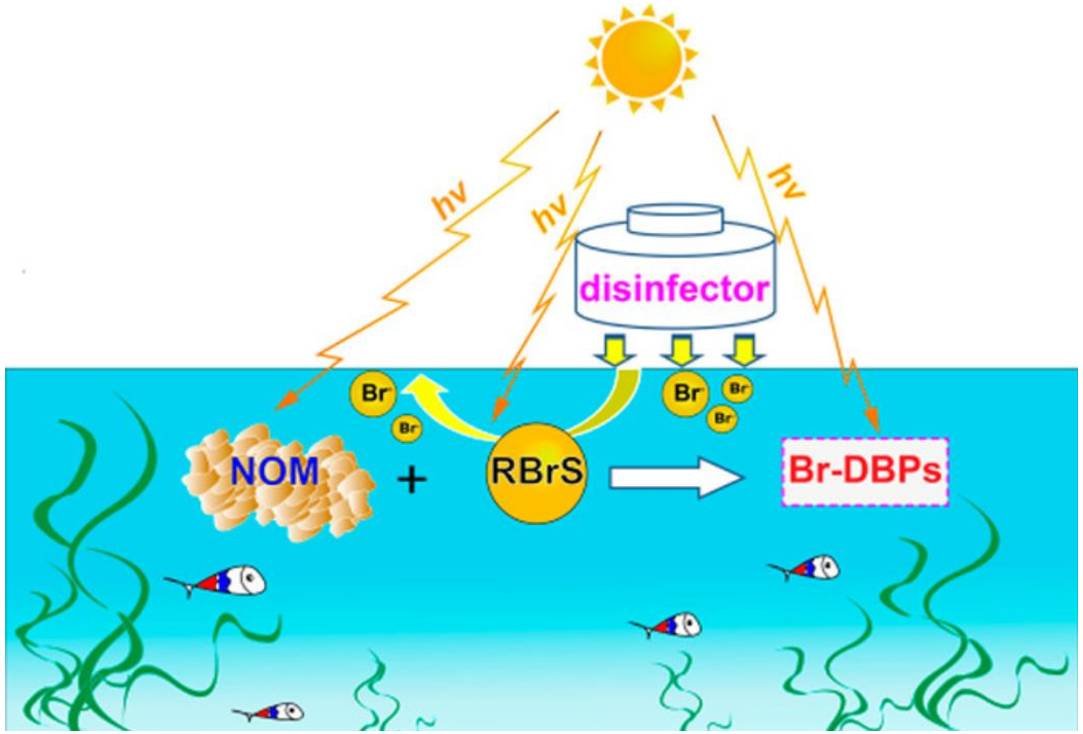
The DOM may be the major consumer of oxidants, and the interaction between DOM and some oxidants (e.g., chlorine, chlorine dioxide, chloramine) could generated halogenated by-products (X-BPs).

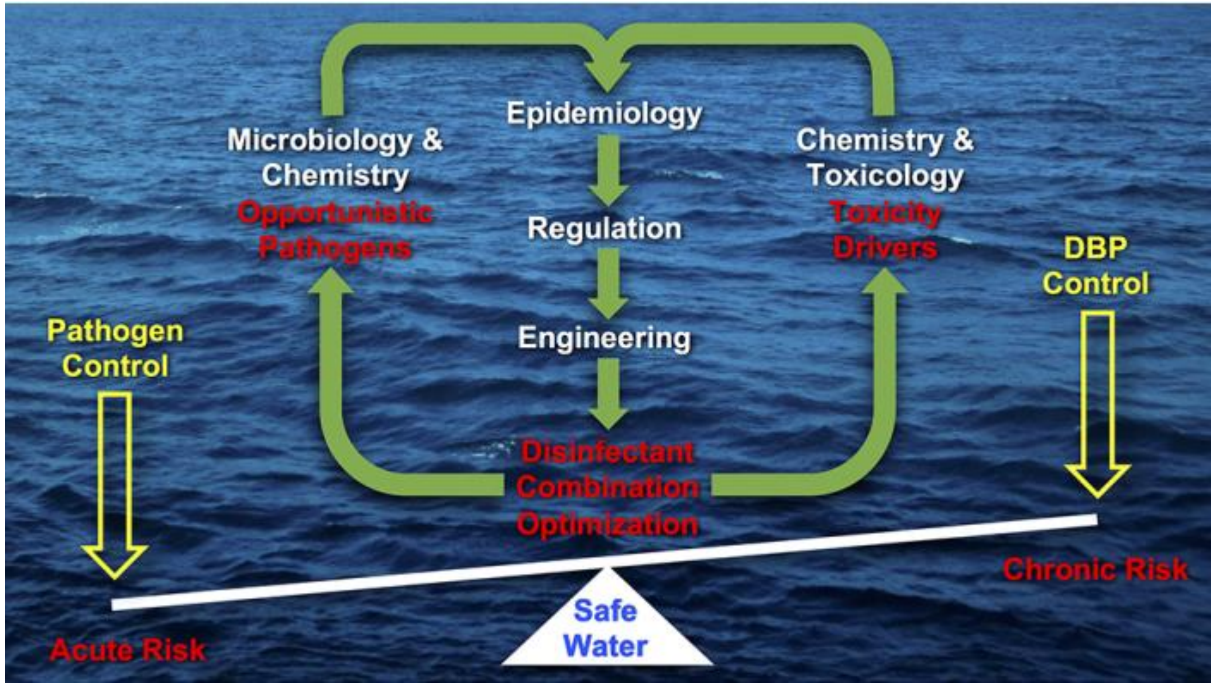
Von Gunten*. *Environ. Sci. Technol.* **2018**, 52, 5062−5075.

Adervse health outcomes of DBPs

Disinfection by-products may be associated with many adverse health outcomes, including bladder cancer and miscarriages.

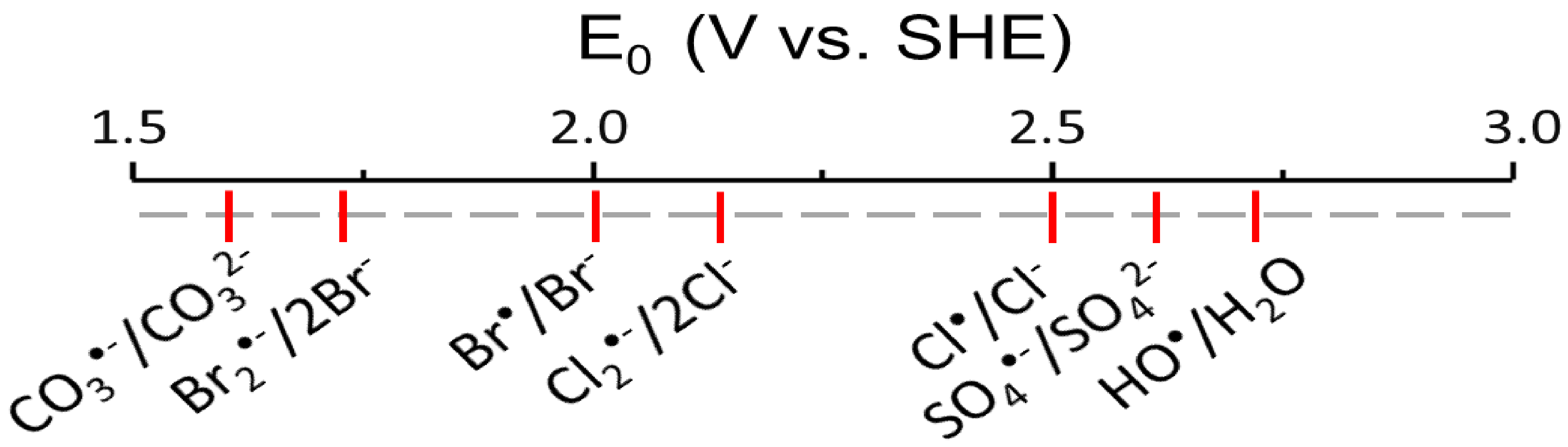
There are strict restrictions on the MCL of halogenated byproducts in the water.

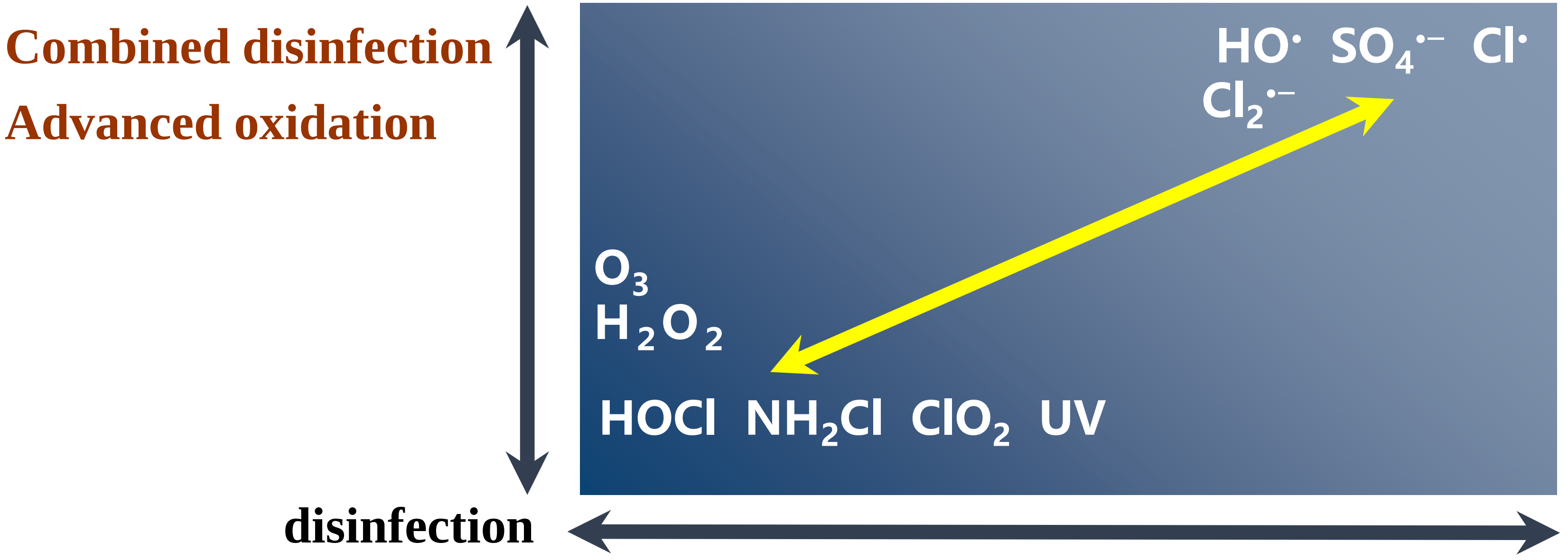




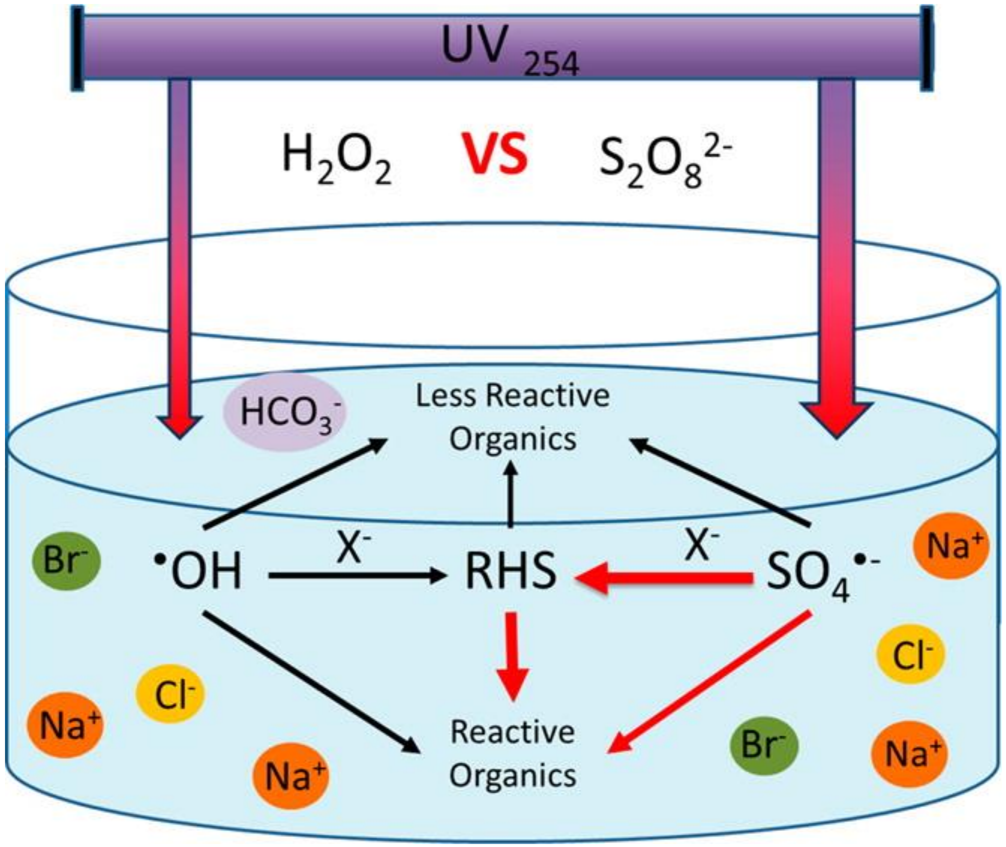
Hu*. *Environ. Sci. Technol.* **2015**, 49, 12, 7218–7226. Li*, Mitch*. *Environ. Sci. Technol.* **2018**, 52, 1681−1689.

The AOPs in Water Treatment





Radicals in AOPs



A scheme of UV-based AOPs

The generation of halogen radicals in $^•OH/SO_4^{•–}$-mediated AOPs in waters containing halide ions.

$HO^• + Cl^–/Br^– \rightleftharpoons ClOH^{•–}/BrOH^{•–}$

$ClOH^{•–}/BrOH^{•–} + H^+ \rightleftharpoons Cl^•/Br^• + H_2O$

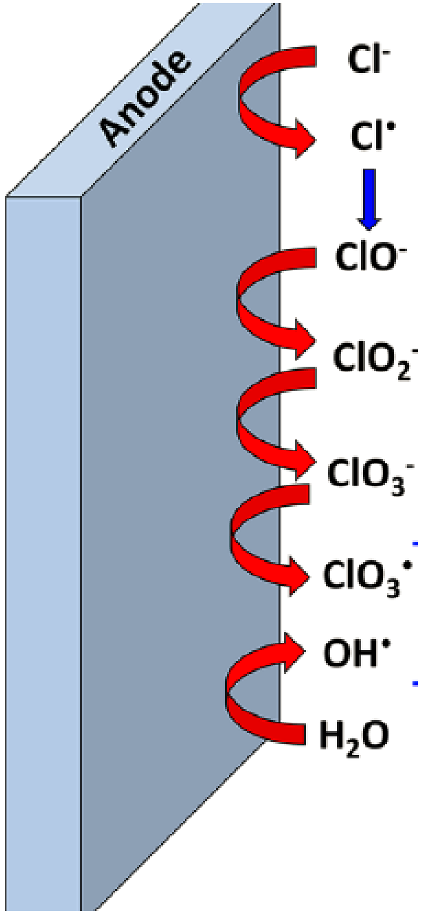
$SO_4^{•-} + Cl^–/Br^– \rightarrow SO_4^{2-} + Cl^•/Br^•$

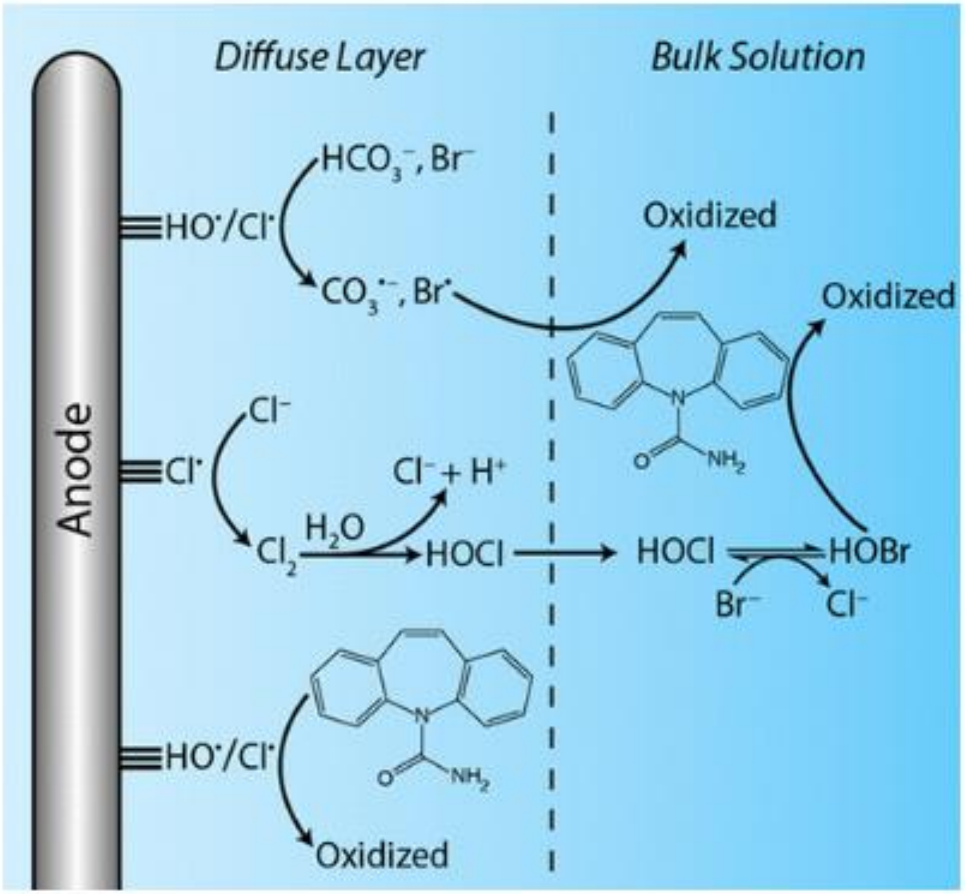
$Cl^• + Cl^– \rightleftharpoons Cl_2^{•–}$

$Br^• + Br^– \rightleftharpoons Br_2^{•–}$ etc.

Yang, Jiang*, Ma*. *Environ. Sci. Technol*. **2015**. 49. 7330-7339. Sun, Huang*. *Environ. Sci. Technol*. **2016**. 50. 13265-13273

Radicals in electrochemical treatment



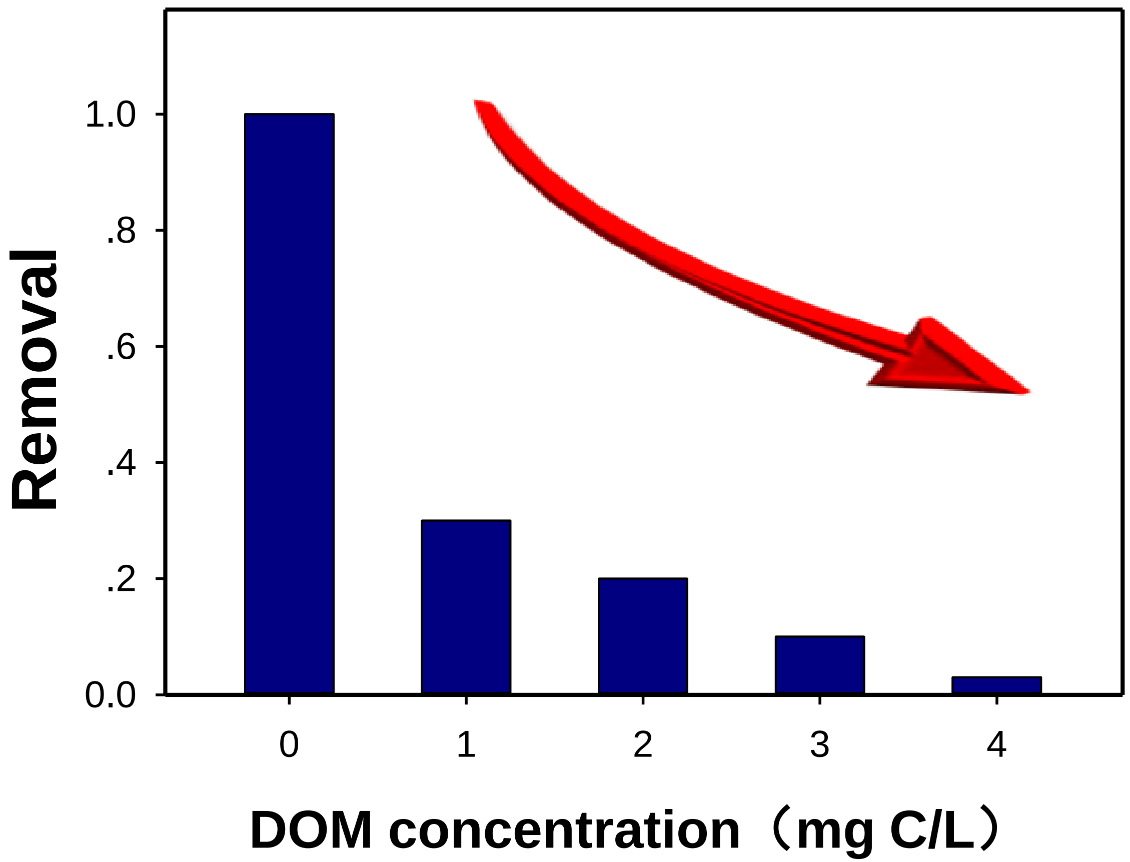


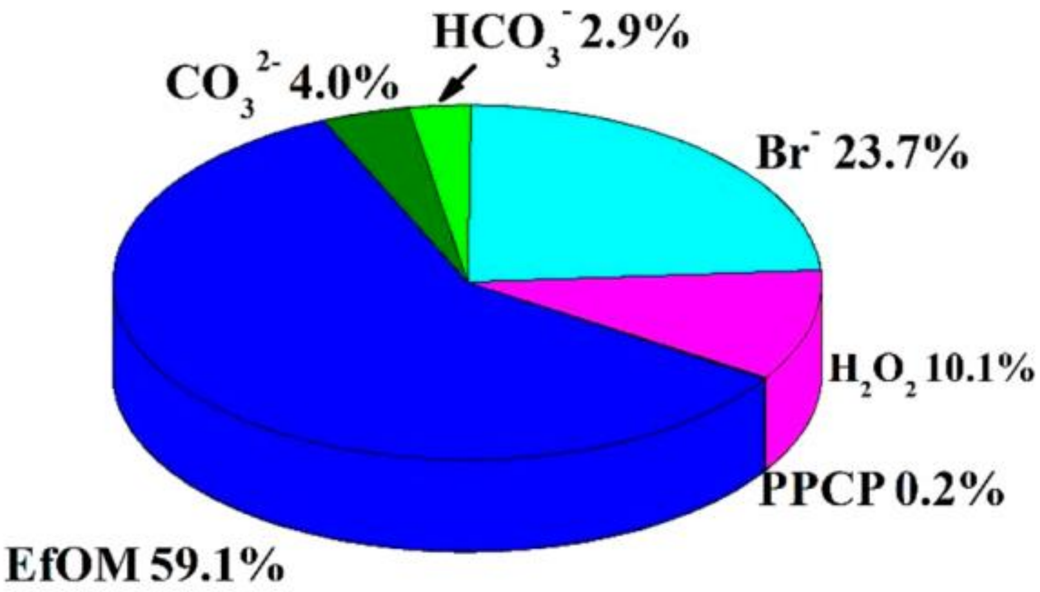
Radicals could be generated on the anode during electrochemical treatments.

Chaplin*. *Acc. Chem. Res.* **2019**, 52, 596−604. Barazesh, Sedlak*. *Environ. Sci. Technol*. **2016**, 50, 10143-10152

The role of DOM in the AOPs

The efficiencies of AOPs are reduced due to the scavenging of radicals by DOM



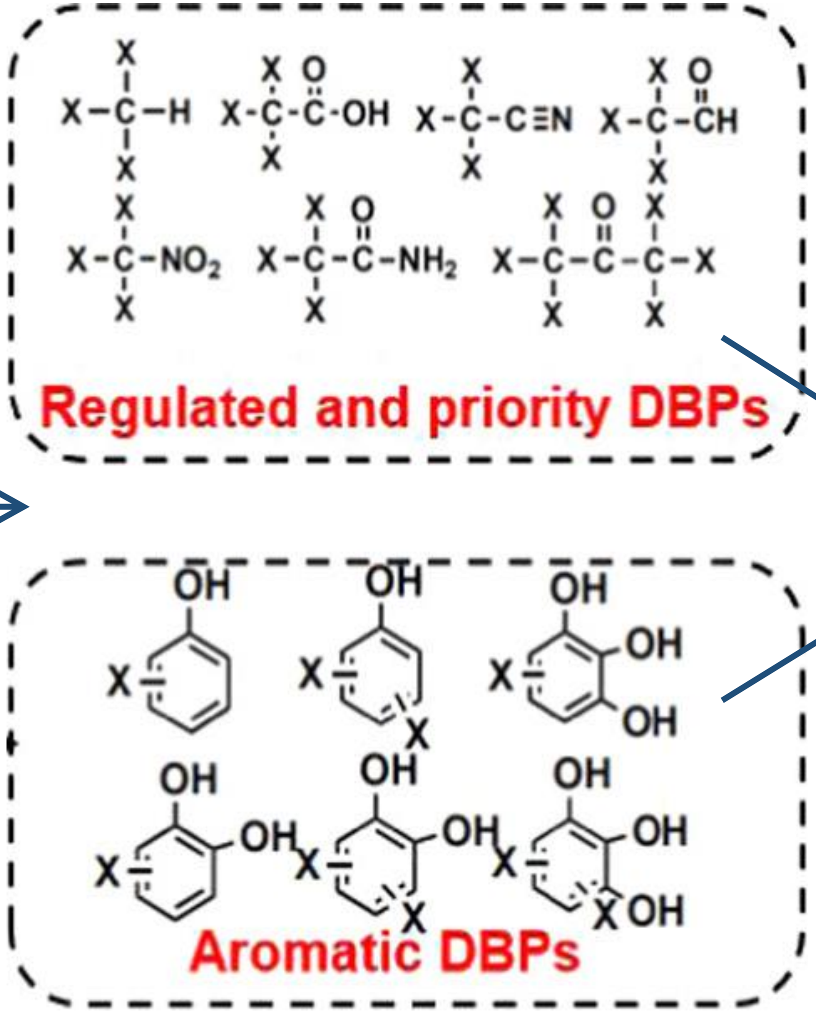


DOM is the main scavenger of •OH.

Lian, Song*. *Environ. Sci. Technol.* **2017**, 51, 2954−2962.

The role of DOM in the AOPs

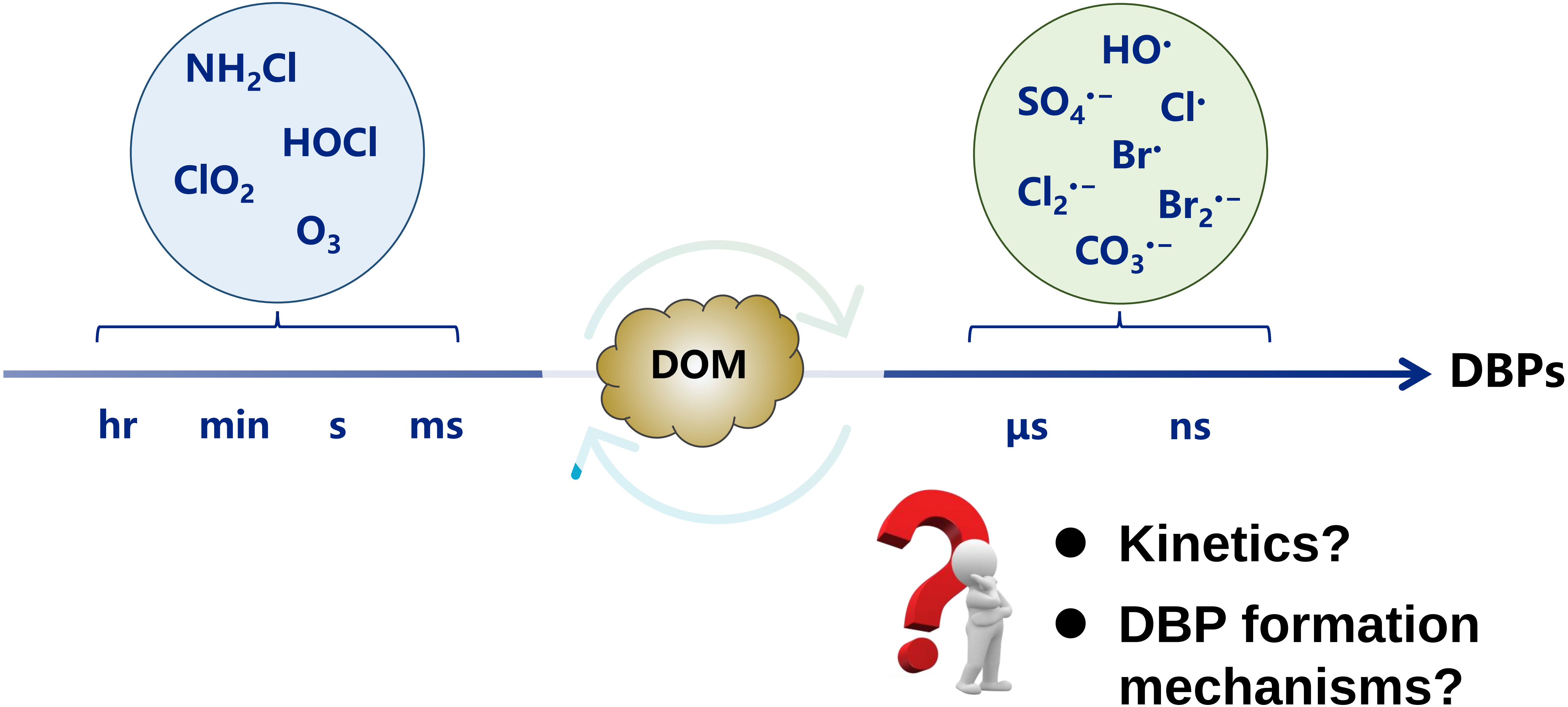
DOM



Transformation byproducts

Sedlak*, von Gunten, ***Science***. 2011, 331, 42; Li*, Mitch*. ***Environ. Sci. Technol.*** 2018, 52, 1681

Radical reactions with DOM and DBP formation

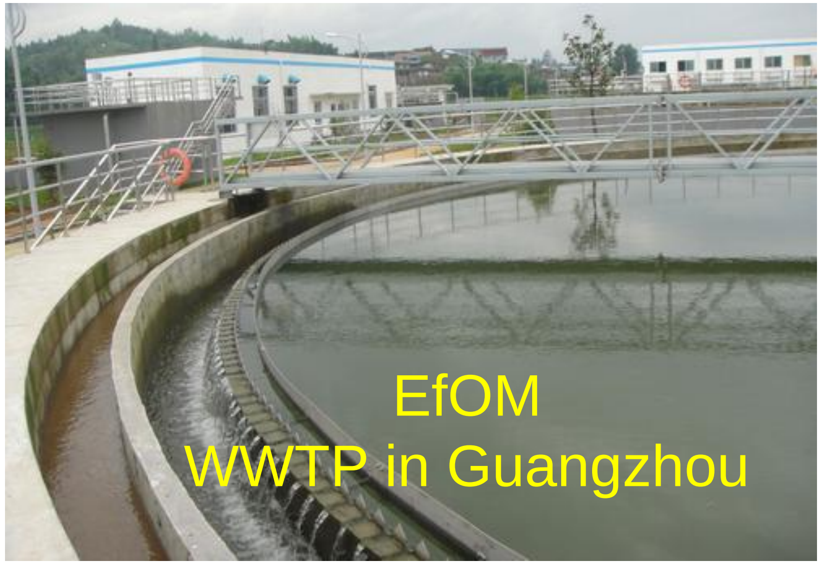


- **Kinetics?**
- **DBP formation mechanisms?**

Methods and Results

DOM with different types and sources

No.	Types
1	RO isolates
2	Fulvic acids
3	Humic acids
4	EfOM
5	Algal OM
6	Hydrophobic/ hydrophilic fractions



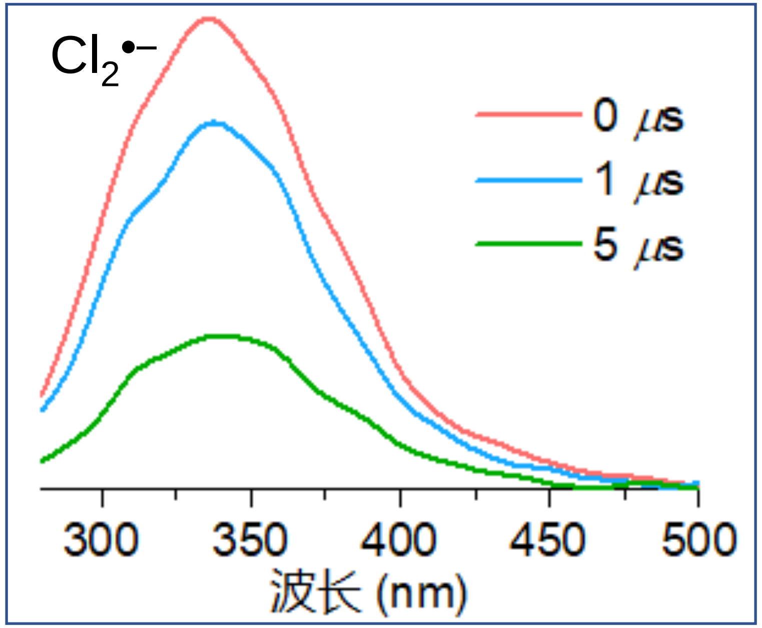
Laser flash photolysis

$$CH_3COCH_2Cl \xrightarrow{hv} Cl^{\bullet}$$

$$S_2O_8^{2-} + Cl^- \xrightarrow{hv} Cl_2^{\bullet -}$$

$$BrCH_2CH_2Br \xrightarrow{hv} Br^{\bullet}$$

$$H_2O_2 + Br^- \xrightarrow{hv} Br_2^{\bullet -}$$



$$S_2O_8^{2-} + Cl^- \xrightarrow{hv} Cl_2^{\bullet -}$$

$$H_2O_2 + Br^- \xrightarrow{hv} Br_2^{\bullet -}$$

Negligible contribution of HOX

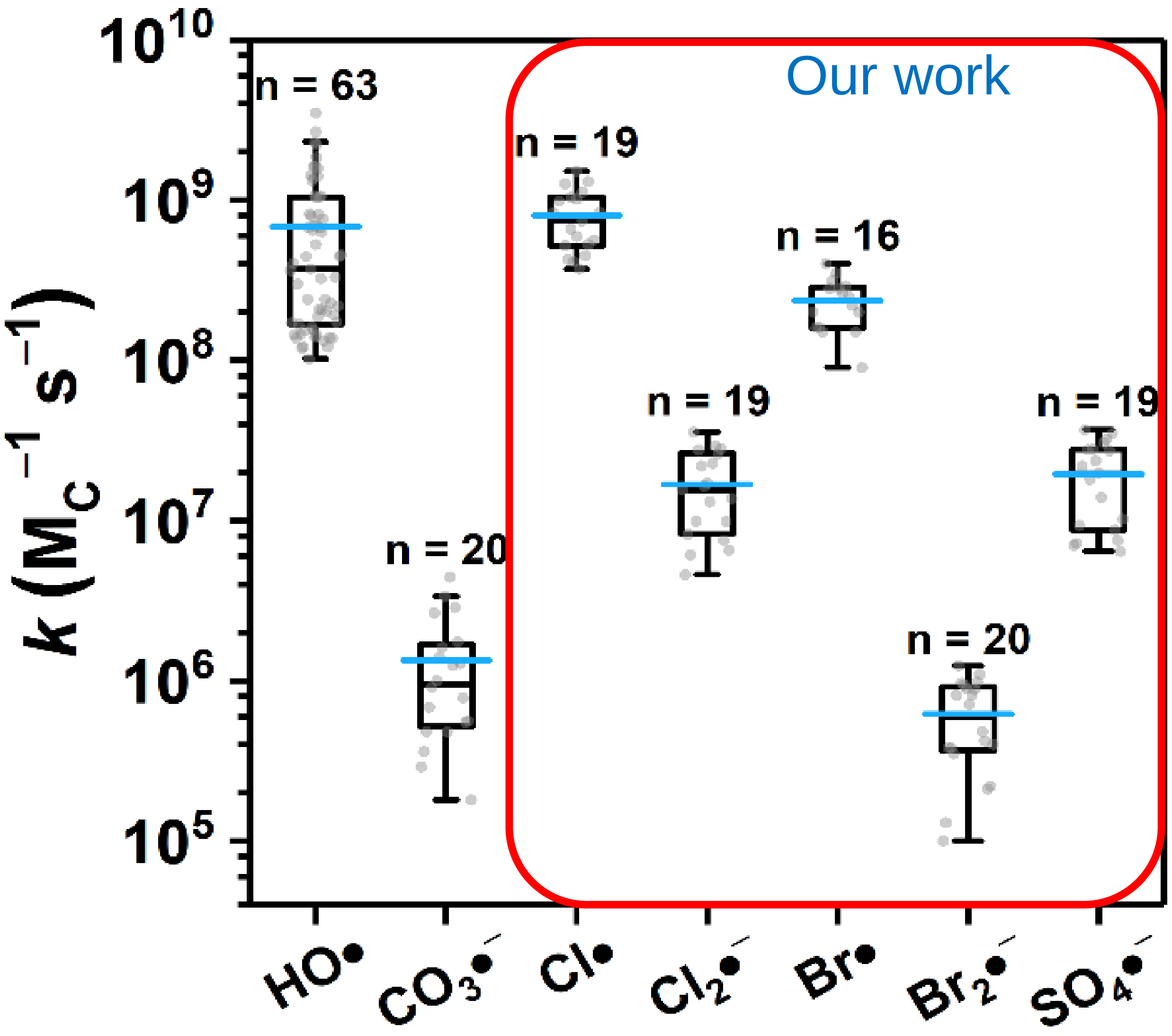
$Br^{\bullet}/Br_2^{\bullet -}$

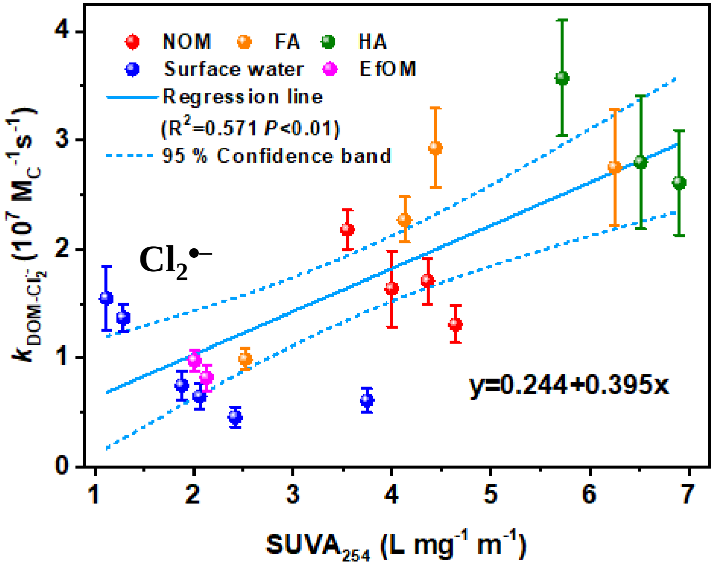
$Cl^{\bullet}$

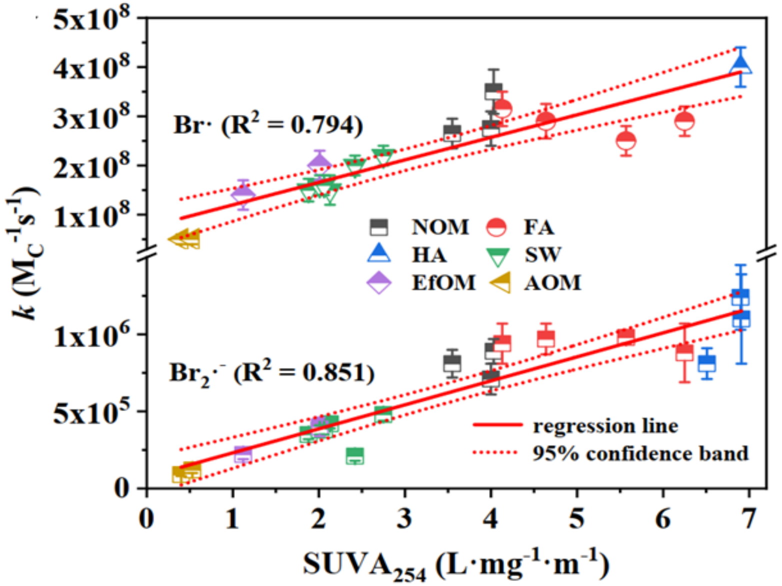
For kinetics experiments

For DBP experiments

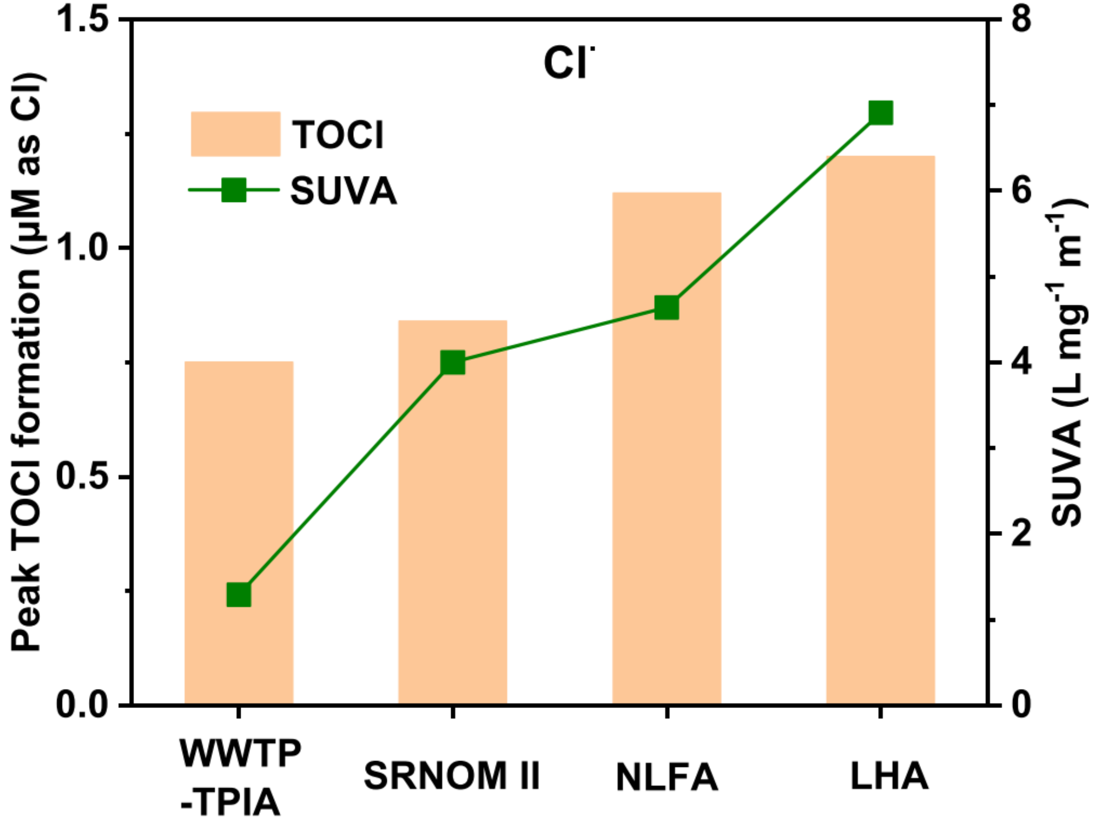
Rate constants of radicals with DOM

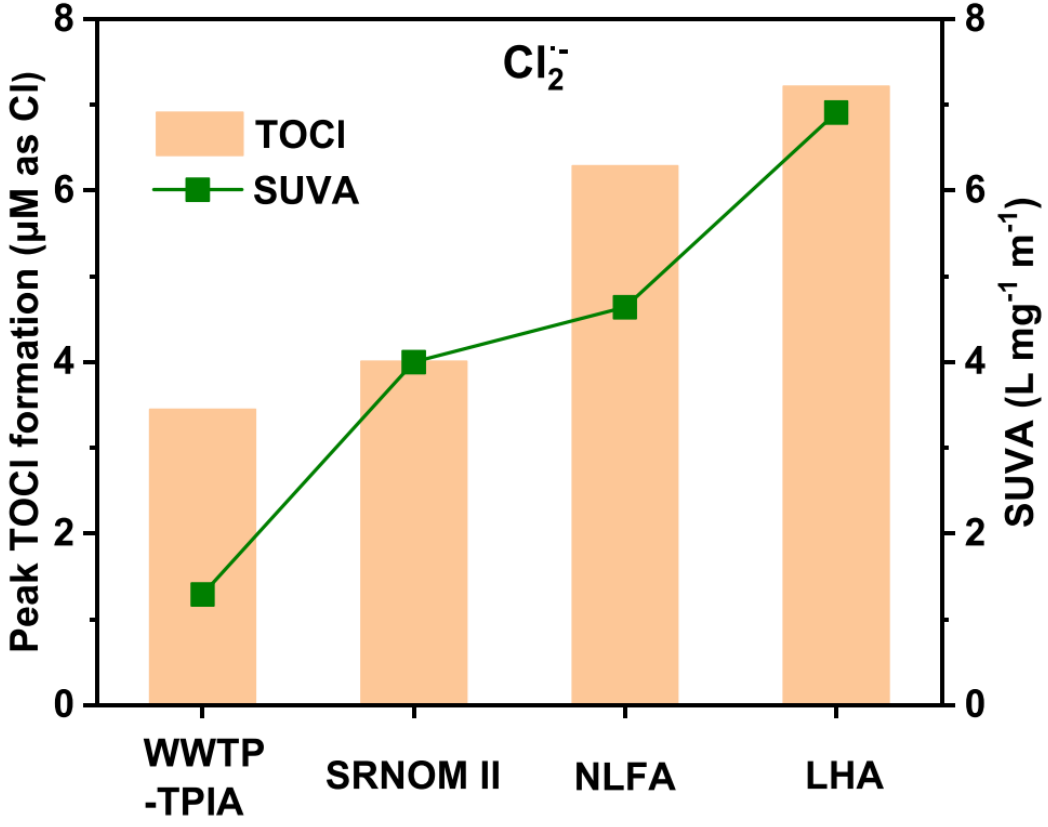






Formation of chlorinated byproducts

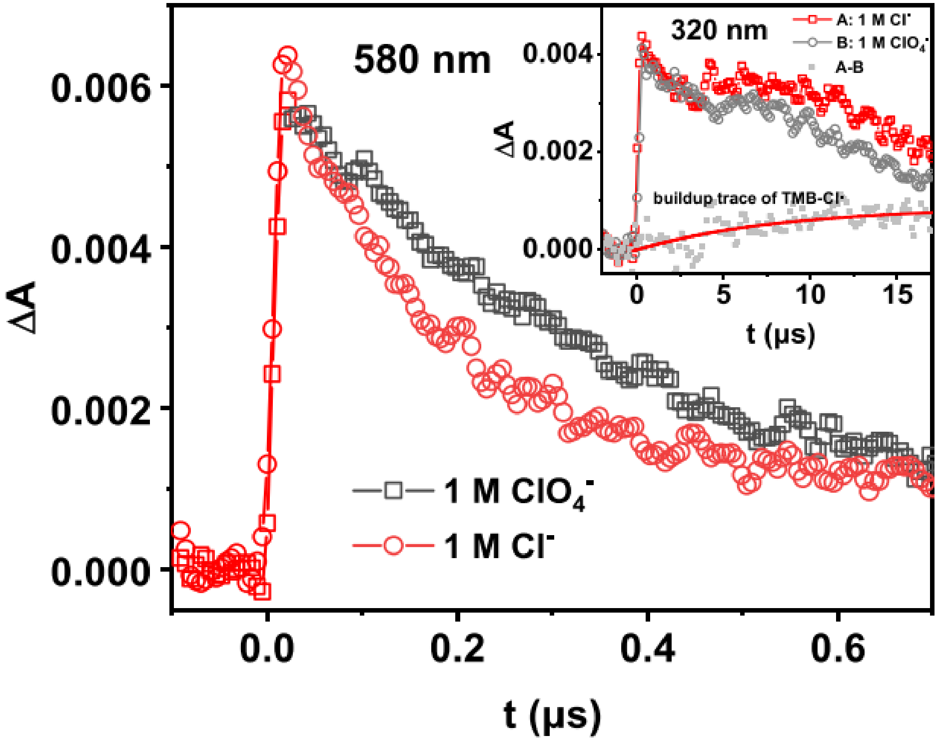


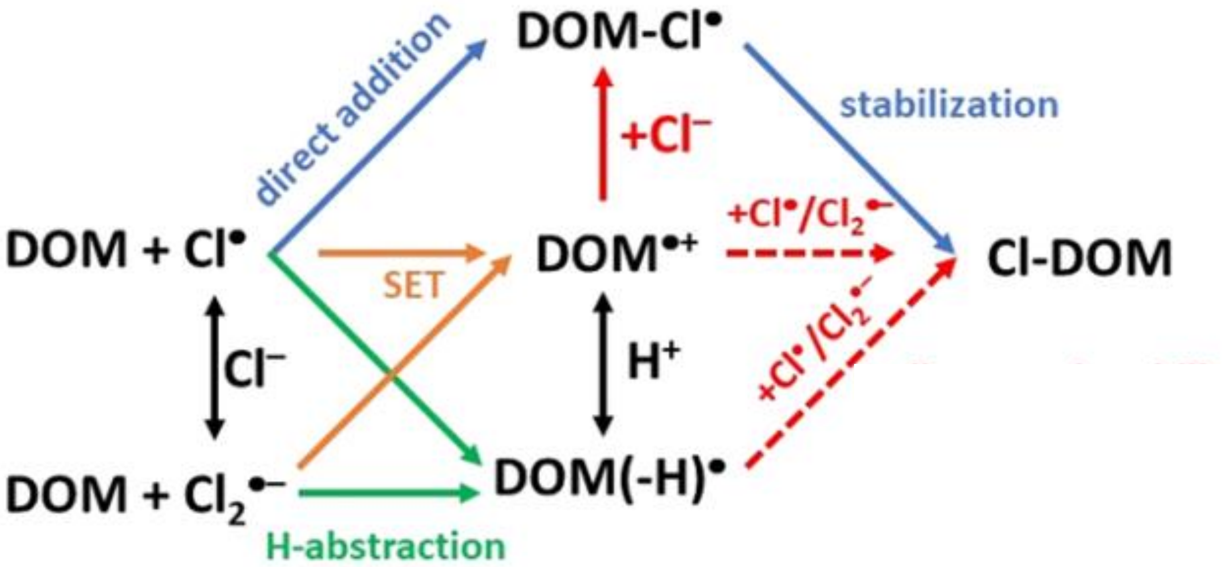


SUVA ↑ TOCl formation ↑

Aromatic moieties of DOM are important precursors of TOCl.

TOCl formation mechanism



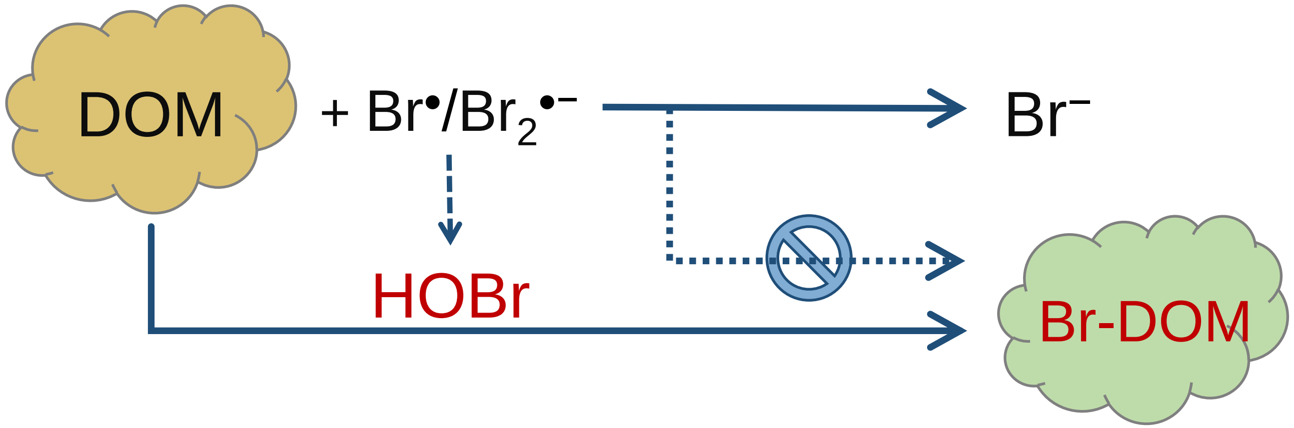


Laser experiments of model compounds

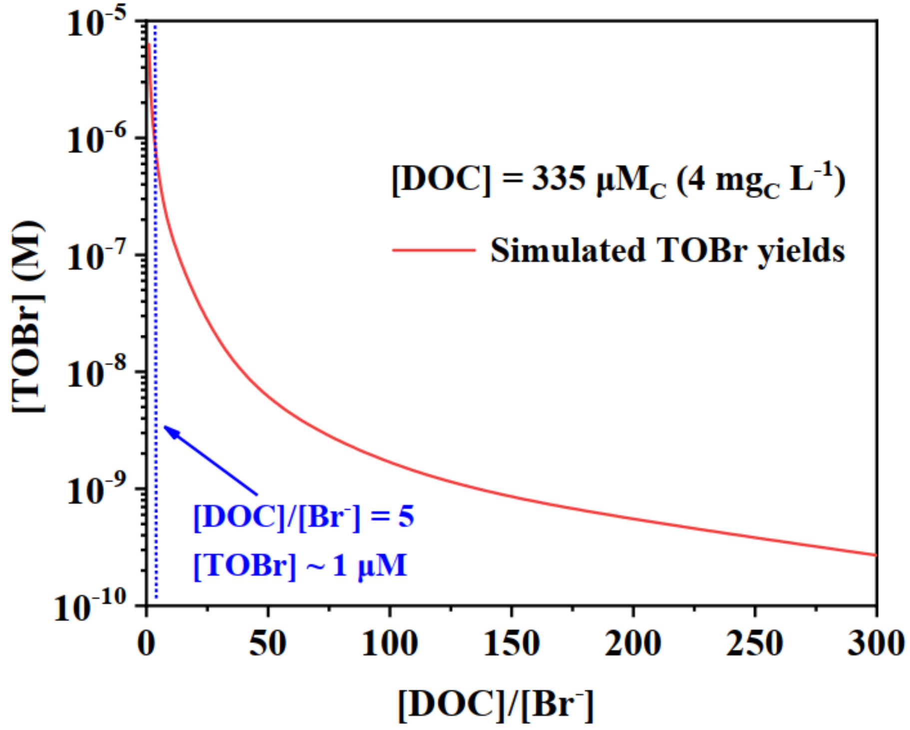
1. Direct incorporation of halogen radicals to DOM
2. Interactions between DOM's intermediates and halogen radicals

Formation of brominated byproducts

Brominated byproducts in AOPs are generated from HOBr, not from $Br^{\bullet}/Br_2^{\bullet-}$



Simulating [HOBr] and predicting the formation of brominated byproducts

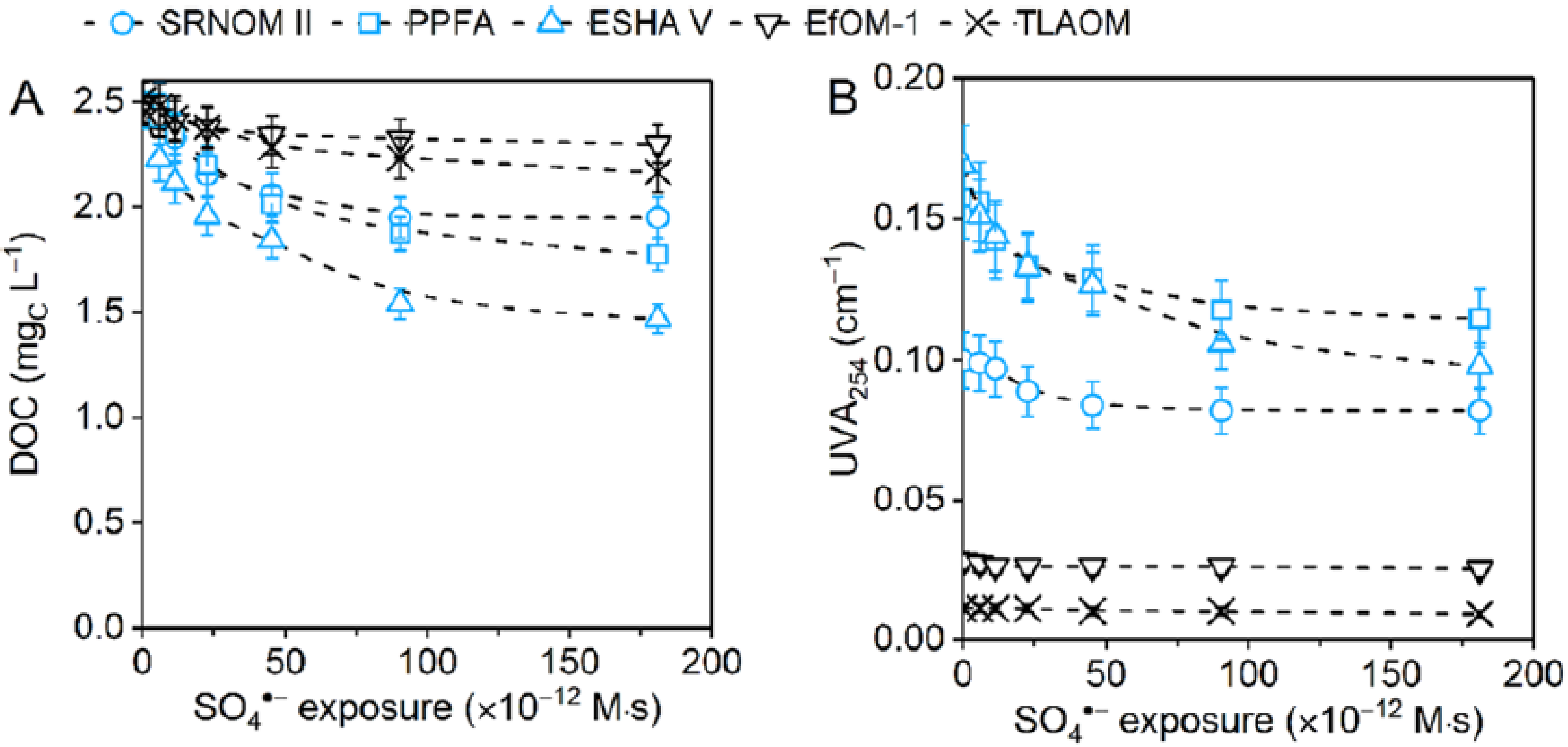


$[DOM]/[Br^-]\uparrow$, brominated byproducts ↓

➢ Guide the control of brominated byproducts in AOPs

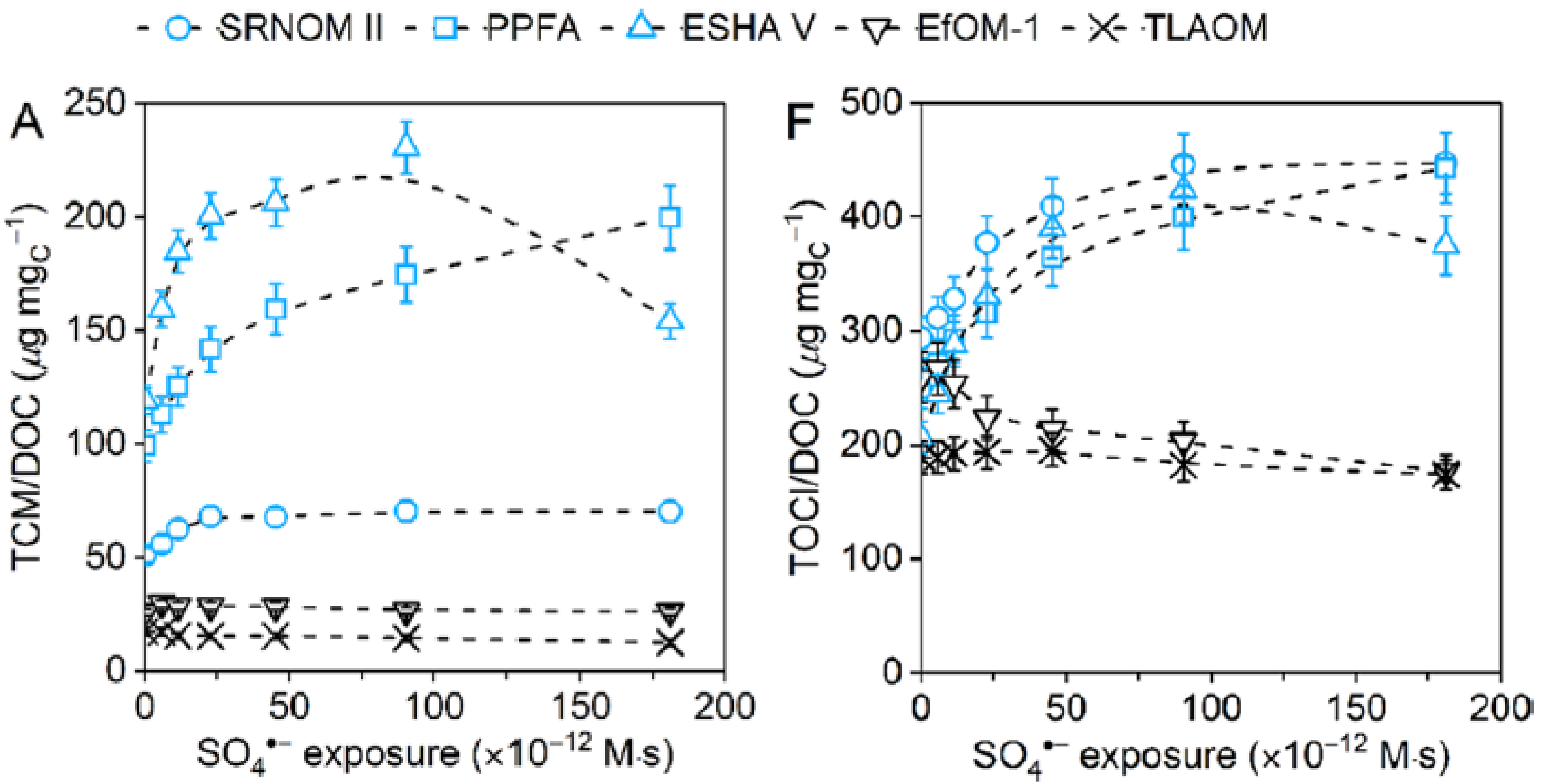
Lei, Y..., Yang, X.*, **Environ. Sci. Technol.,** 2021, 55, 689. Lei, Y..., Yang, X.*, **Environ. Sci. Technol.,** 2022, 56, 5189.

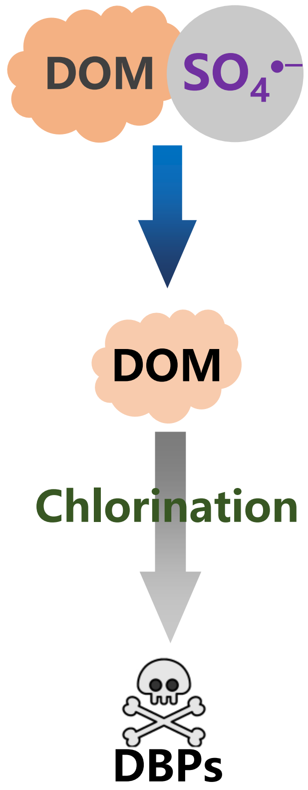
$SO_4^{\bullet-}$-Induced Transformation of DOM



- $SO_4^{\bullet-}$ oxidation results in higher reductions in DOC and UV_{254} for high aromatic DOM.

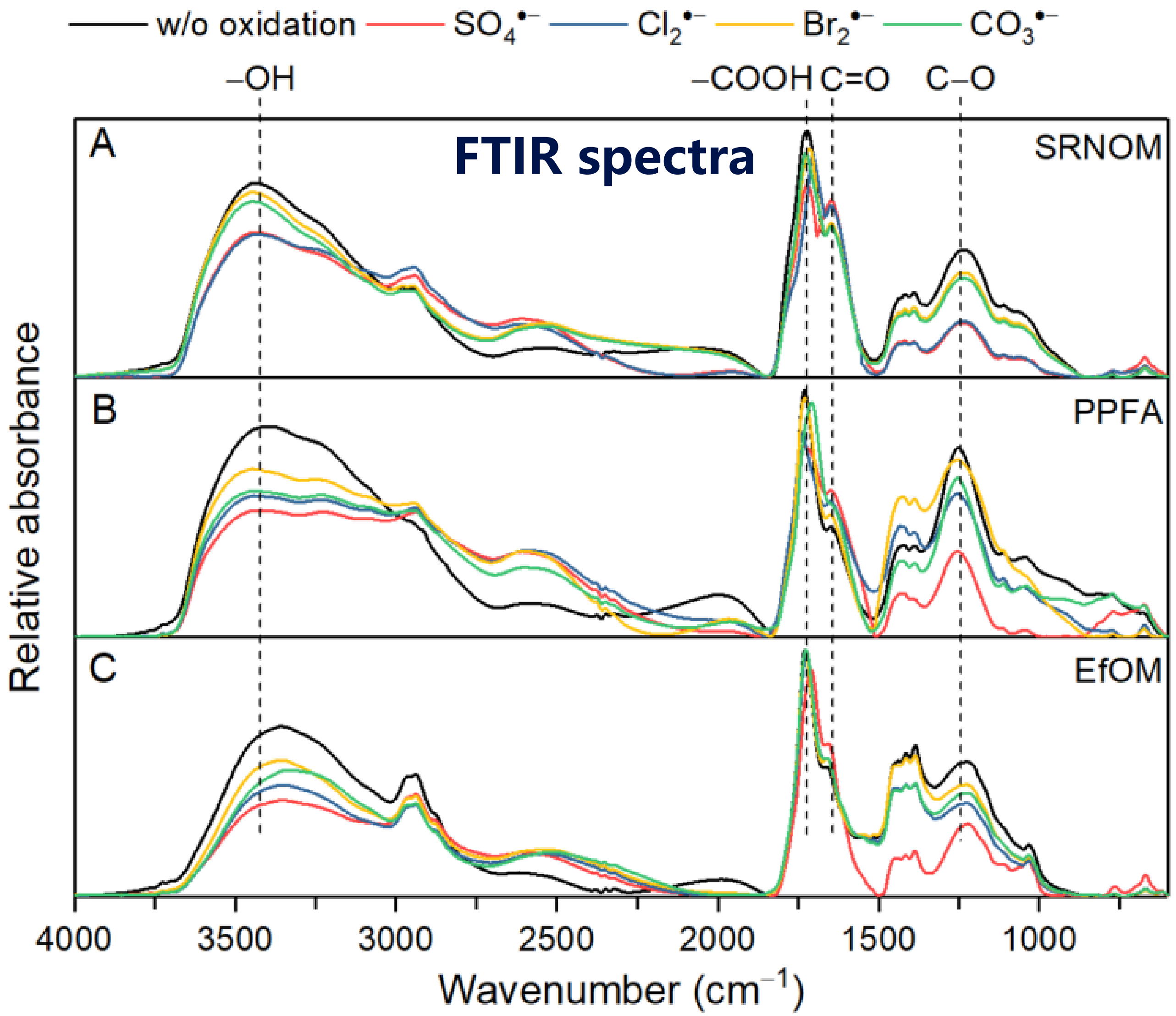
$SO_4^{\bullet-}$-Induced Transformation of DOM





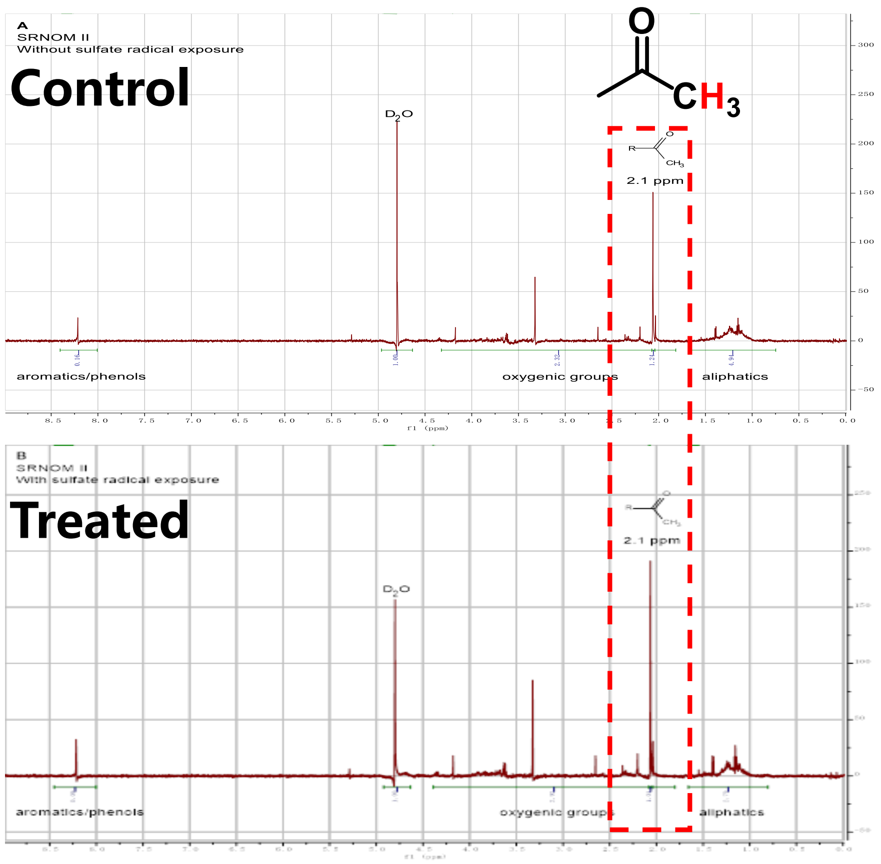
➤ $SO_4^{\bullet-}$ oxidation results in more DBP precursors for high aromatic DOM.

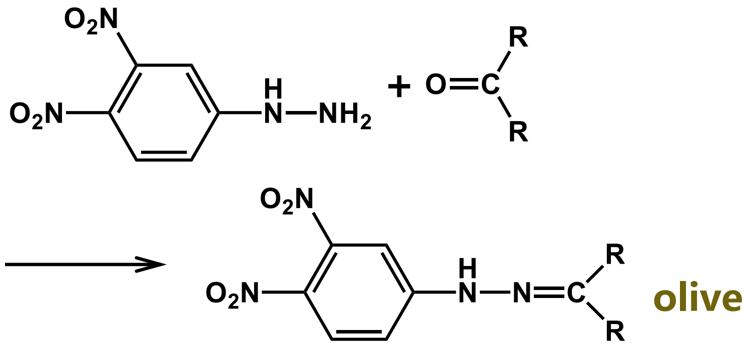
Radical-Induced DOM Transformation



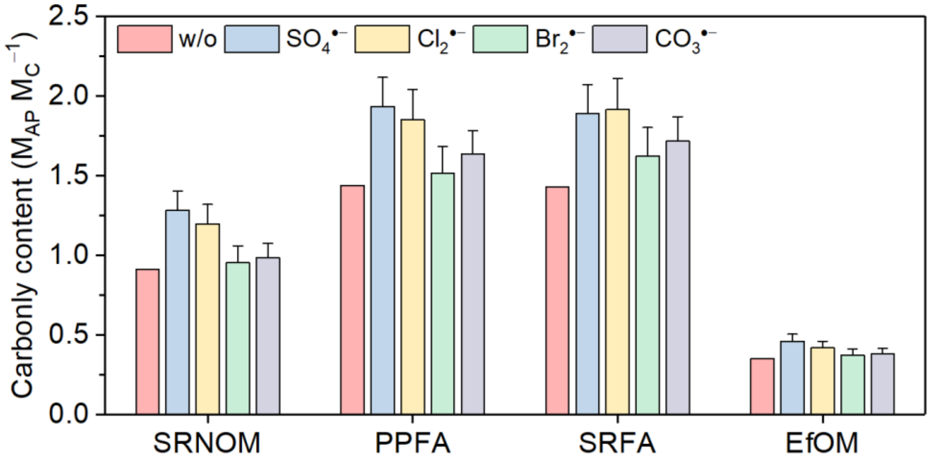
◆ One-electron oxidants decrease phenolic/hydroxyl groups and increase carbonyl groups.

Radical-Induced DOM Transformation





2,4-dinitrophenylhydrazine colorimetry



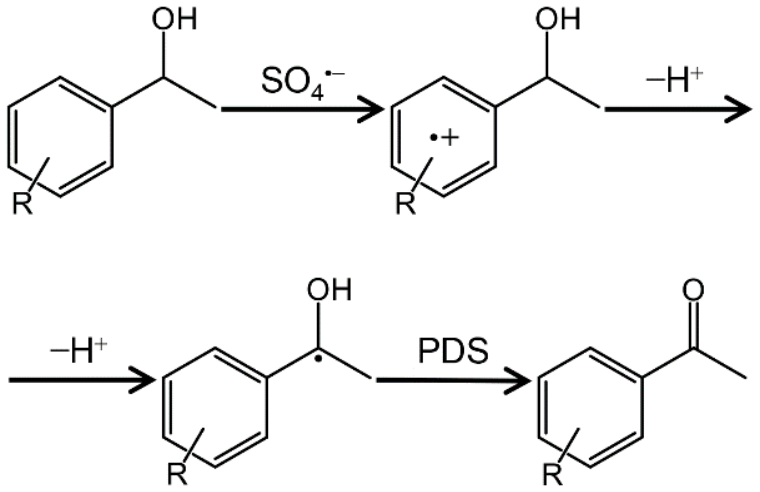
NMR spectra

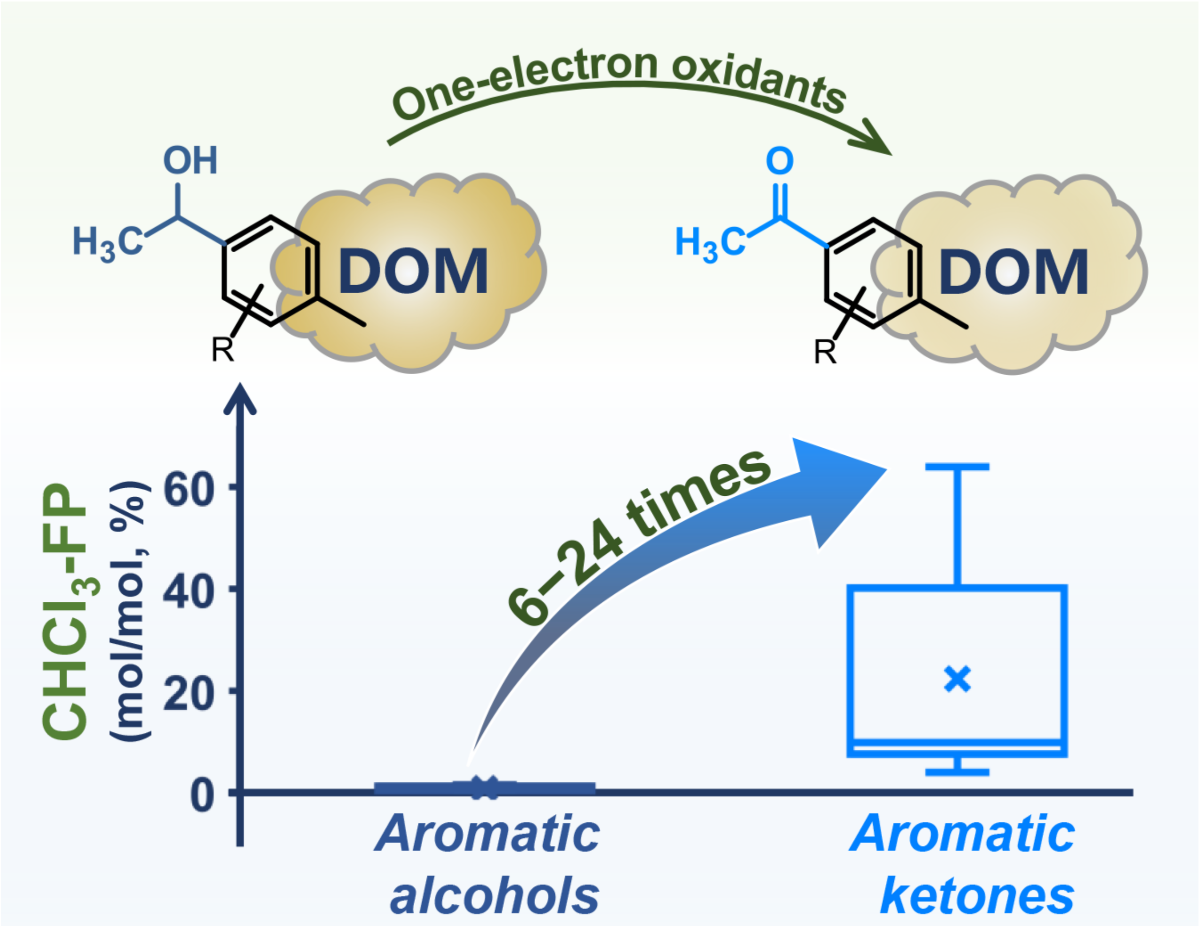
carbonyl groups

- One-electron oxidants increase carbonyl group in DOM.

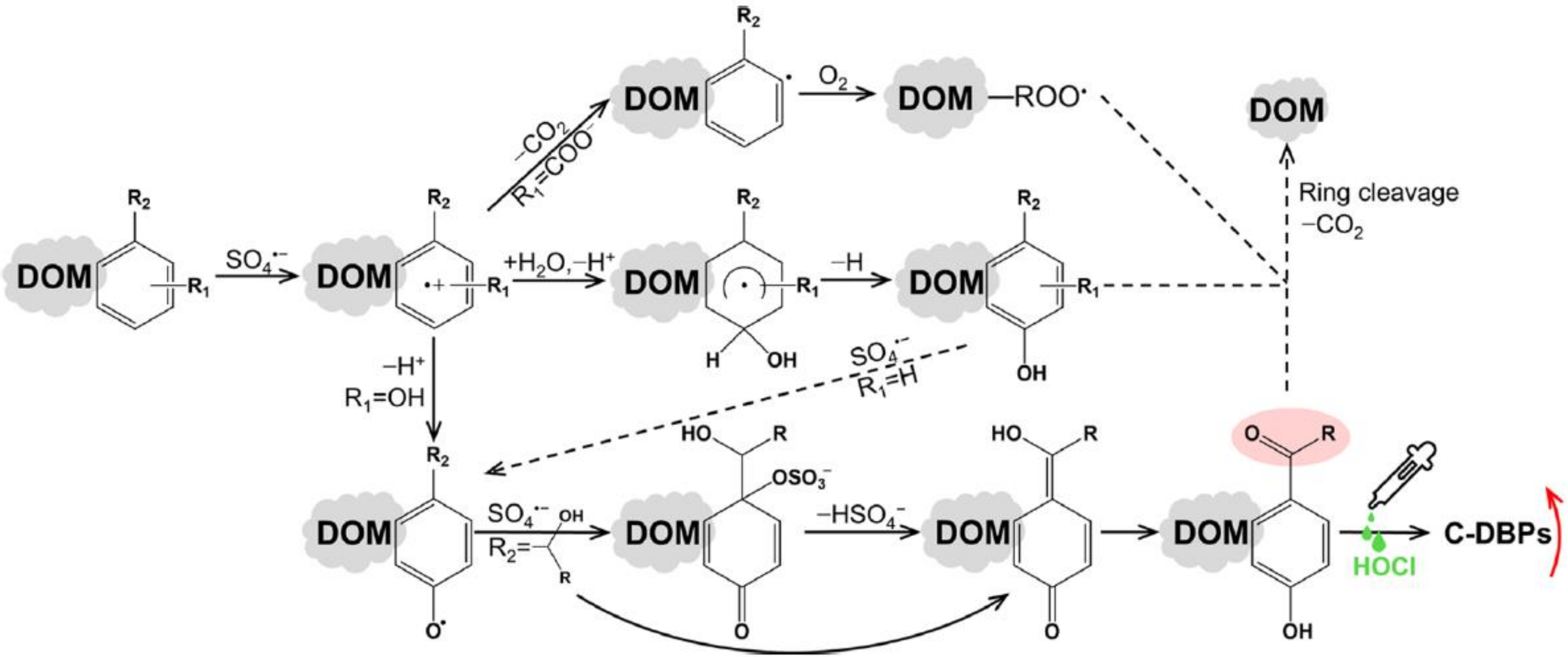
Radical-Induced DOM Transformation

◆ **Comparison of DBP formation from aromatic alcohols and aromatic ketones**





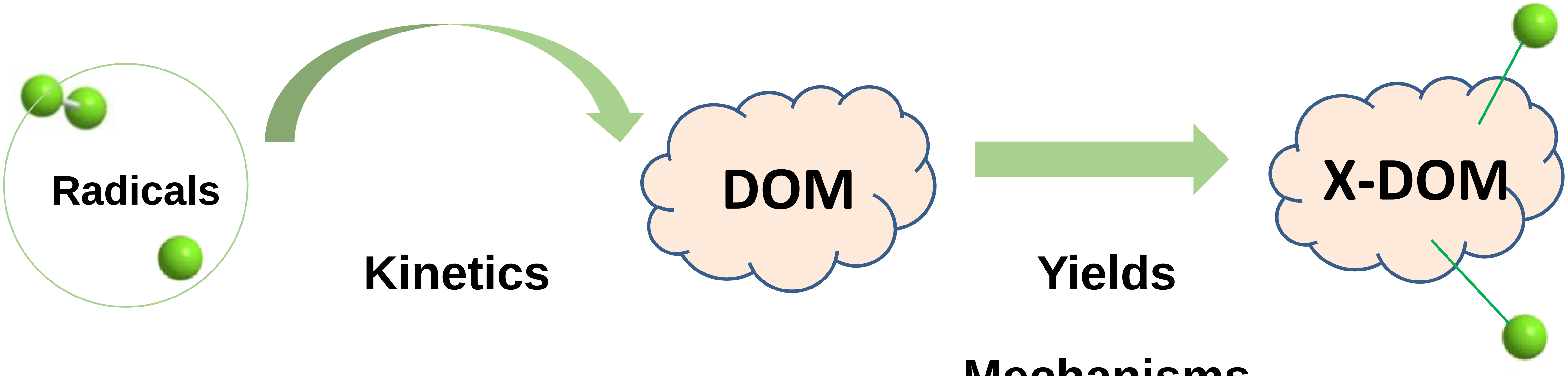
Radical-Induced DOM Transformation



Lei, X..., Yang, X.*, **Environ. Sci. Technol.,** 2023, 57, 18597.

Lei, X..., Yang, X.*, **Water Res.,** 2024, 249, 121011.

Conclusions

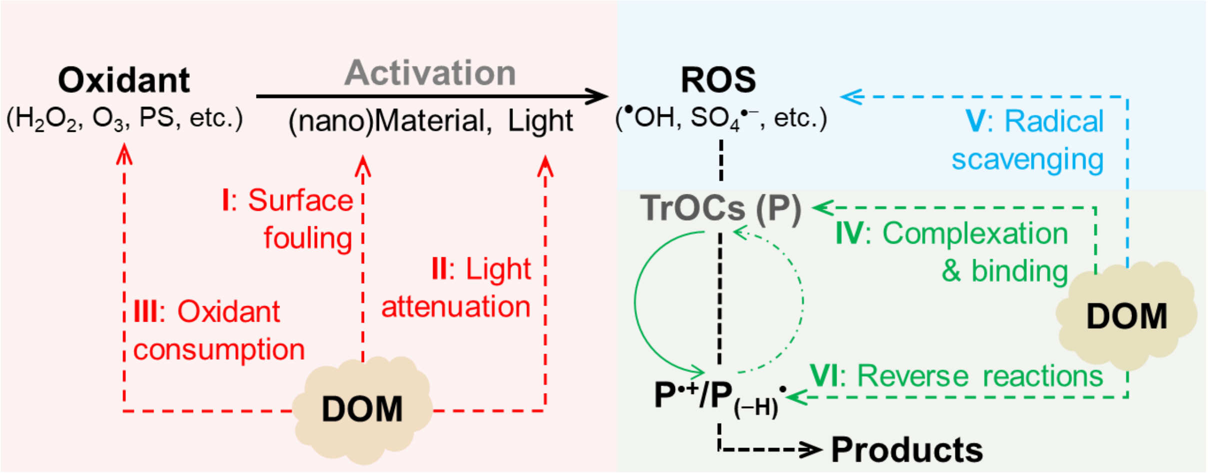


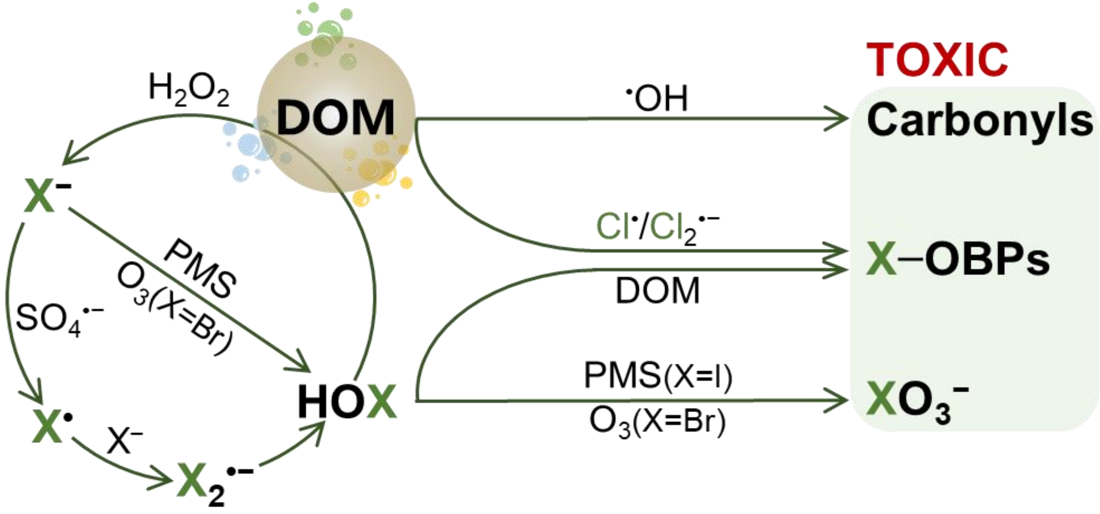
(1) Method for radicals

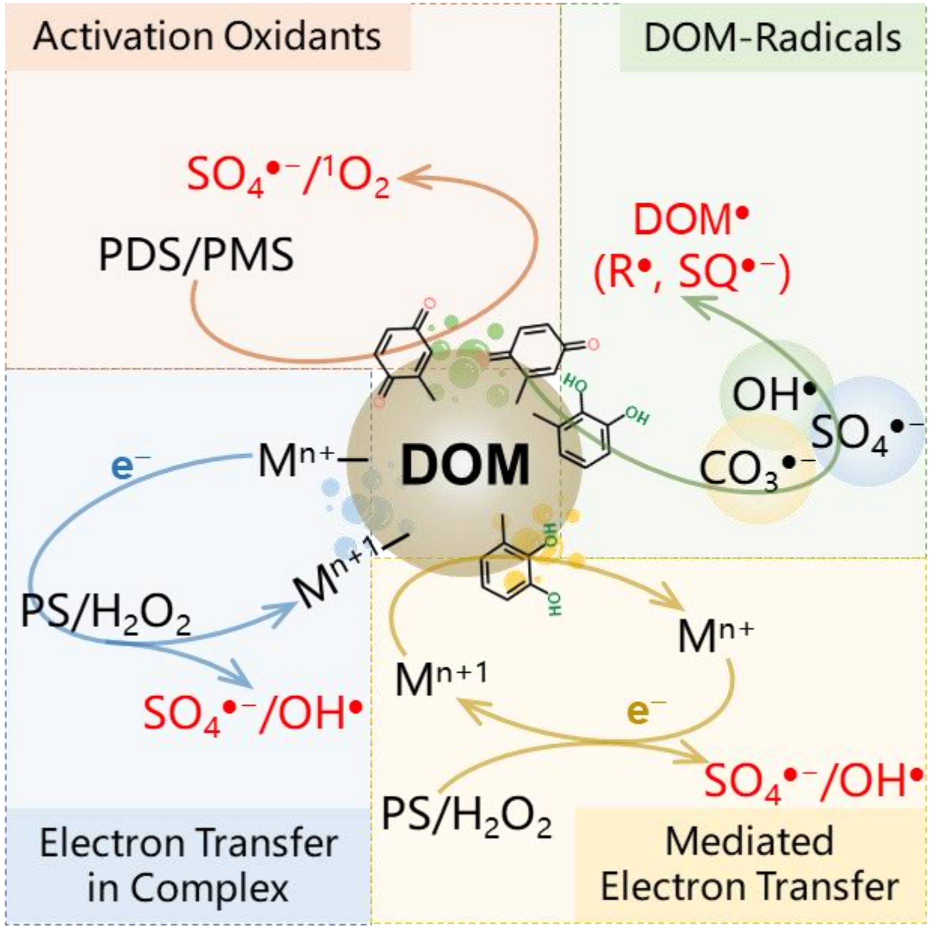
(2) Kinetics data

(3) Mechanisms DOM transformation byproducts

More about DOM







Yang, X.*, Rosario-Ortiz, F. ... Westerhoff, P., Multiple roles of dissolved organic matter in advanced oxidation processes. **Environ. Sci. Technol.**, 2022, 56, 11111−11131. (ESI highly cited paper, EST best paper award)

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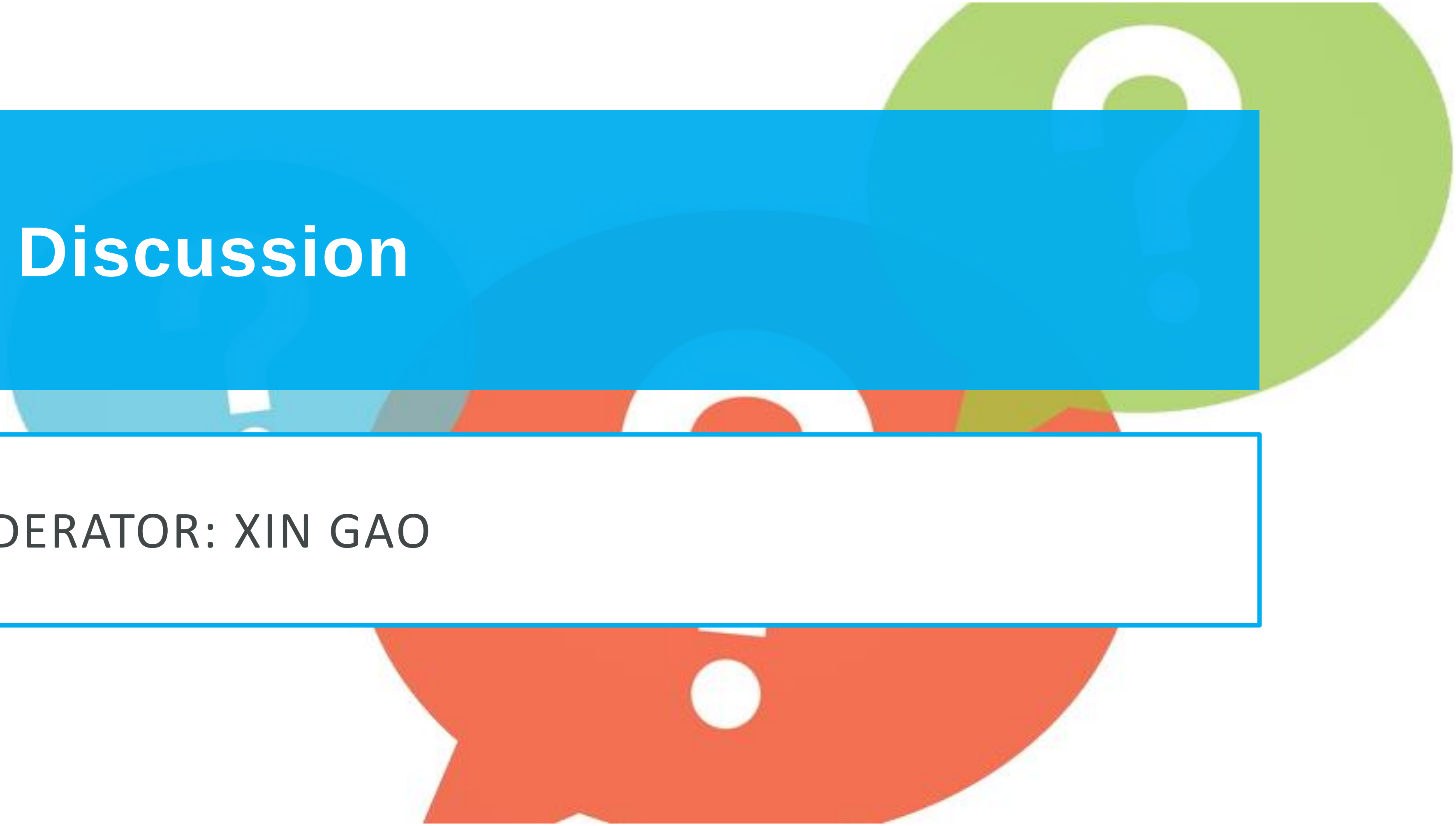
Website：https://sese.sysu.edu.cn/yangxin

Email: yangx36@mail.sysu.edu.cn

Thank you!

the international water association

Q&A Discussion



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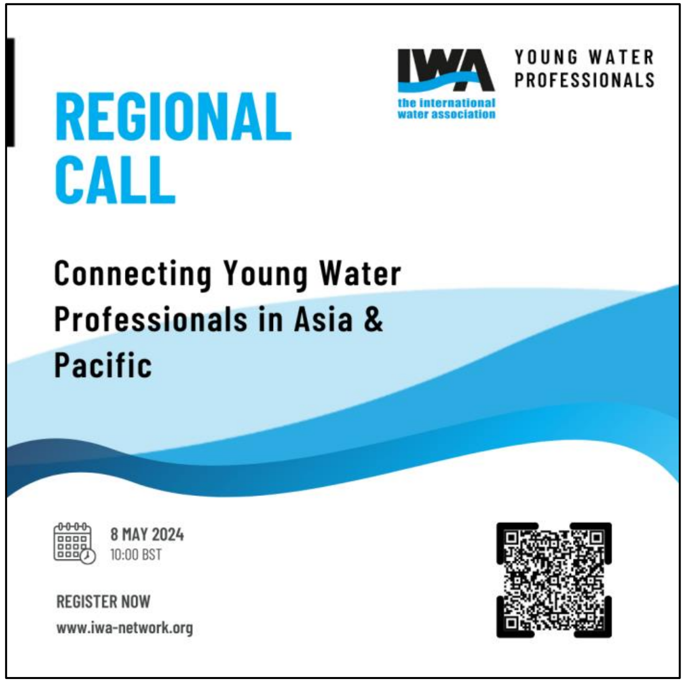

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