Effect of benzophenone type UV filters on photodegradation of co-existing sulfamethoxazole in water

Authors: Dilini Kodikara, Zhongyu Guo and Chihiro Yoshimura *

Department of Civil and Environmental Engineering, Tokyo Institute of Technology, Tokyo 152-8552, Japan.

*Corresponding author: yoshimura.c.aa@m.titech.ac.jp

Supplementary materials

Table S1. Equations and calculations used in chemical actinometry experiment [53].

Equation	Variable	
$\boldsymbol{\phi_{PNA} = 0.29[PYR]_0 + 0.00029}$	ϕ_{PNA}	Quantum yield of PNA (mol/Einstein)
	$[pyr]_0$	Initial PYR concentration (1×10^{-2} M)
$\boldsymbol{E^0_{p,tot} = \frac{k'[PNA]_0 l}{1000\phi \sum_\lambda \rho_\lambda (1 - 10^{-\varepsilon_\lambda l[PNA]_0}) \Delta\lambda}}$	$E^0_{p,tot}$	Photon irradiance (Einstein/cm^2.s)
	k'	PNA degradation rate constant (s^{-1}), experimentally calculated for each tube position
	l	Optical path length (1.256 cm)
	ρ_λ	Relative spectral photon irradiance (for each wavelength 280-400 nm, from the lamp manufacturer)
	ε_λ	PNA molar absorption coefficient at each wavelength (/M.cm) from (1)
	$[PNA]_0$	Initial PNA concentration (1×10^{-5} M)
	$\Delta\lambda$	Wavelength resolution (1 nm)

Table S2. Results of the data analysis of indirect photodegradation induced by the BPs in the experimental system. "-" indicates not applicable and "n.d." indicates that the calculation was not applied due to the inhibition of the photodegradation of SMX at those BP or BP3 ratios.

[BP or BP3]/ [SMX]	**SMX + BP**					**SMX + BP3**				
	S	$k_{obs\_(BP)}$ $(h^{-1}) \times 10^{-2}$	k_{d+s} $(h^{-1}) \times 10^{-2}$	k_{ind} $(h^{-1}) \times 10^{-3}$	k_{ind} as a percentage of $k_{obs\_(BP)}$	*S*	$k_{obs\_(BP3)}$ $(h^{-1}) \times 10^{-2}$	k_{d+s} $(h^{-1}) \times 10^{-2}$	k_{ind} $(h^{-1}) \times 10^{-3}$	k_{ind} as a percentage of $k_{obs\_(BP3)}$
0.00	-	-	2.23	-	-	-	-	2.23	-	-
0.10	0.998	3.03	2.22	8.11	26.7	0.992	2.93	2.21	7.18	24.5
0.25	0.993	3.34	2.21	11.30	33.8	0.985	3.03	2.19	8.40	27.7
0.30	0.993	2.39	2.21	1.77	7.4	n.d.	n.d.	n.d.	n.d.	n.d.
0.40	0.995	2.49	2.22	2.73	11.0	n.d.	n.d.	n.d.	n.d.	n.d.
0.50	0.991	2.39	2.21	1.82	7.6	0.980	2.25	2.18	0.64	2.8
0.60	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
0.75	0.992	2.27	2.21	0.61	2.7	n.d.	n.d.	n.d.	n.d.	n.d.
0.90	0.993	2.54	2.21	3.31	13.0	n.d.	n.d.	n.d.	n.d.	n.d.
1.00	0.990	2.41	2.21	2.04	8.5	n.d.	n.d.	n.d.	n.d.	n.d.

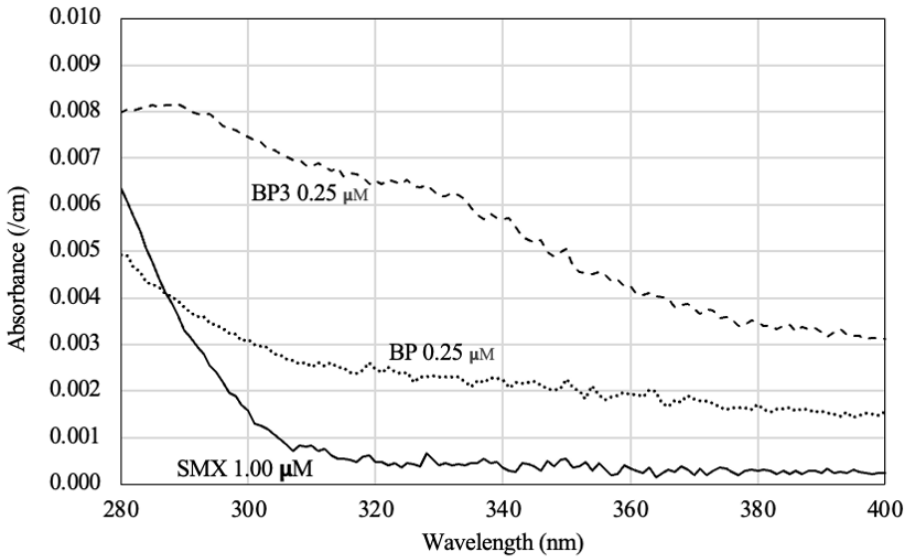

Figure S1. UV absorbance spectra from 280 nm to 400 nm for 1.00 µM of SMX and 0.25 µM of BP and BP3 measured using UV-vis spectrophotometer (UV1800, Shimadzu, Japan).