Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts

Occurrence and Removal of Benzotriazole Ultraviolet Stabilizers in a Wastewater Treatment Plant in China

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Table S1. Technical parameters of the WWTP investigated in this study

	Serving population	Loading (m^3/day)	Hydraulic Retention Time (hour)	Sludge Retention Time (day)	BOD_5, in/out (mg/L)	COD_{cr}, in/out (mg/L)
WWTP	**2,000,000**	**300,000**	**16**	**10**	**175/3**	**451/11**

Table S2: Optimized parameters for BZT-UVs

Analyte	Parent ion (m/z)	Daughter ion (m/z)	Cone voltage (V)	Collision voltage (V)	Retention Time (min)	MQL (ng/g, ng/mL)
UV-P	**226**	**120/107**	**35**	**21/19**	**6.46**	**0.45**
UV-329	**324**	**212/57**	**40**	**23/28**	**12.38**	**0.61**
UV-234	**448**	**370/119**	**40**	**40/40**	**15.36**	**0.15**
UV-326	**316**	**260/57**	**40**	**20/27**	**15.76**	**0.60**
UV-327	**358**	**302/57**	**40**	**24/32**	**17.14**	**0.75**
UV-328	**353**	**282/71**	**40**	**23/29**	**16.40**	**0.35**
UV-320	**324**	**268/212**	**40**	**21/28**	**14.90**	**0.75**
IS	**266**	**238/119**	**35**	**24/24**	**10.79**	**0.35**

MQL, Method quantification limit, calculated as a signal-to-noise ratio of 10

Table S3: Mass flux (mean values, g/d) of dissolved and adsorbed BZT-UVs in water samples from each sampling sites

	UV-P		UV-234		UV-329		UV-326		UV-328		Total BZTs	
	Aqueous phase	TSS	Aqueous phase	TSS	Aqueous phase	TSS	Aqueous phase	TSS	Aqueous phase	TSS	Aqueous phase	TSS
Primary Influent	**10.4**	**22.3**	**1.47**	**73.9**	**2.89**	**65.6**	**3.19**	**62.1**	**2.96**	**55.2**	**20.9**	**279**
Primary Effluent	**7.61**	**8.41**	**1.38**	**15.2**	**2.11**	**33.5**	**2.33**	**25.8**	**1.86**	**31. 6**	**15.3**	**114**
Anaerobic Effluent	**6.94**	**12.3**	**0.92**	**21.1**	**1.16**	**38.9**	**0.98**	**34.6**	**1.51**	**23.5**	**11.5**	**130**
Anoxic-Oxic Effluent	**6.77**	**16.8**	**0.87**	**30.9**	**0.75**	**33.8**	**1.06**	**39.8**	**1.94**	**17.7**	**11.4**	**140**
Secondary Effluent	**3.93**	**0.25**	**0.70**	**0.23**	**0.75**	**0.45**	**0.75**	**0.45**	**1.02**	**0.31**	**7.15**	**1.69**
Final Effluent	**3.14**	**0.22**	**0.21**	**1.21 $\times10^{-3}$**	**0.75**	**6.91 $\times10^{-3}$**	**0.75**	**1.91 $\times10^{-2}$**	**0.82**	**1.51 $\times10^{-3}$**	**5.67**	**2.47 $\times10^{-1}$**
Primary sludge	**17.2**		**32.9**		**55.2**		**33.2**		**24.3**		**163**	
Secondary sludge	**10.4**		**22.4**		**32.9**		**27.0**		**27.7**		**120**	

Table S4: Concentrations of target BZT-UVs in primary and secondary sludge (ng/g d.w.)

	Primary sludge	**Secondary sludge**
UV-P	203	265
UV-329	388	448
UV-234	649	565
UV-326	391	542
UV-328	286	508

Table S5: Physical-chemical properties of BZT-UVs calculated by EPA suite 4.1

	Water solubility (mg/L)	**Log K_{ow}**
UV-P	25.59	4.31
UV-329	0.168	6.21
UV-234	1.65×10^{-3}	7.67
UV-326	0.684	5.55
UV-328	1.48×10^{-2}	7.25

Table S6: Removal percentages (%) of each treatment unit of five detected BZT-UVs

	Primary clarification	Anaerobic tank	Secondary treatment unit	Secondary clarification	Advanced treatment
UV-P	50.9	-19.9	-0.50	78.4	19.6
UV-329	48.0	-12.8	3.31	96.9	36.7
UV-234	78.0	-33.0	-8.71	96.1	77.3
UV-326	56.9	-26.3	13.3	96.1	36.1
UV-328	42.6	25.1	21.4	93.2	37.9

Table S7: Comparison between model calculation results and data from field samples

		UV-P	UV-329	UV-234	UV-326	UV-328
Sludge adsorption (%)	**EPI suite calculation**	45.4	92.1	93.2	88.1	93.2
	Results from samples	84.6	80.8	117	92.3	89.3
Total removal efficiency (%)	**EPI suite calculation**	45.8	92.9	94.0	88.9	93.9
	Results from samples	89.7	98.9	99.7	98.8	98.6
Sludge adsorption/ Total removal efficiency (%)	**EPI suite calculation**	99.1	99.1	99.1	99.1	99.3
	Results from samples	94.3	81.7	117	93.4	90.6

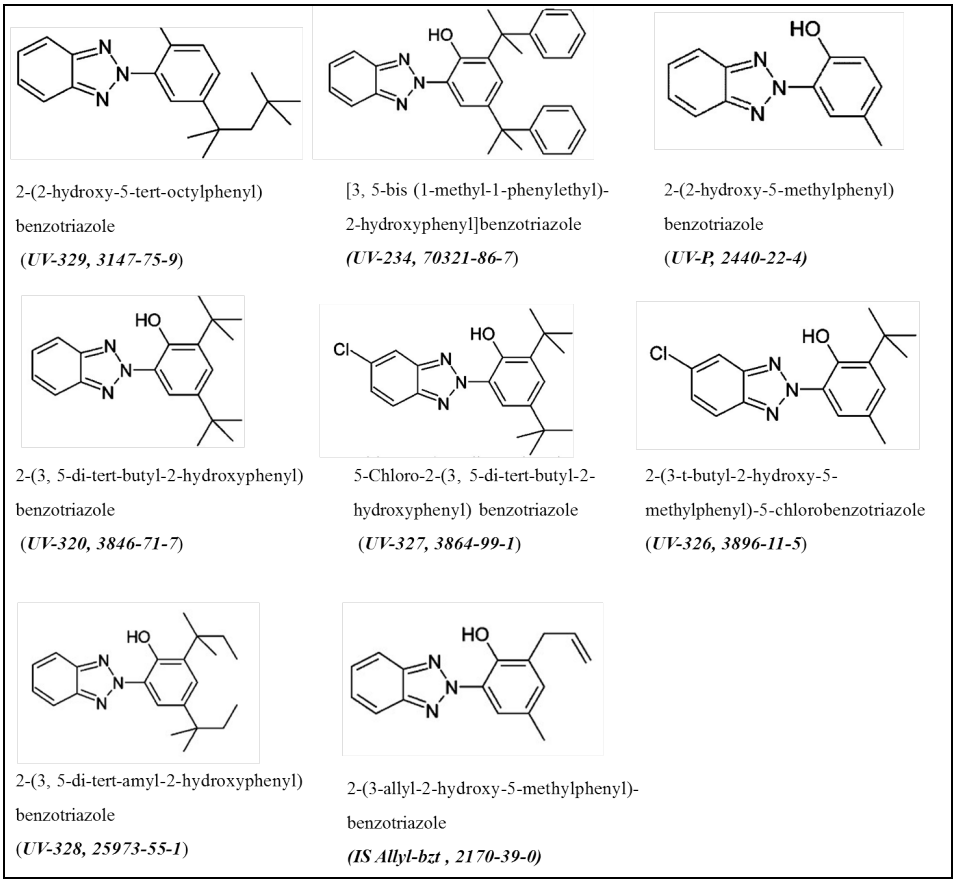

Figure S1 Chemical name, acronym, structure and other information of BZT-UV analogues.

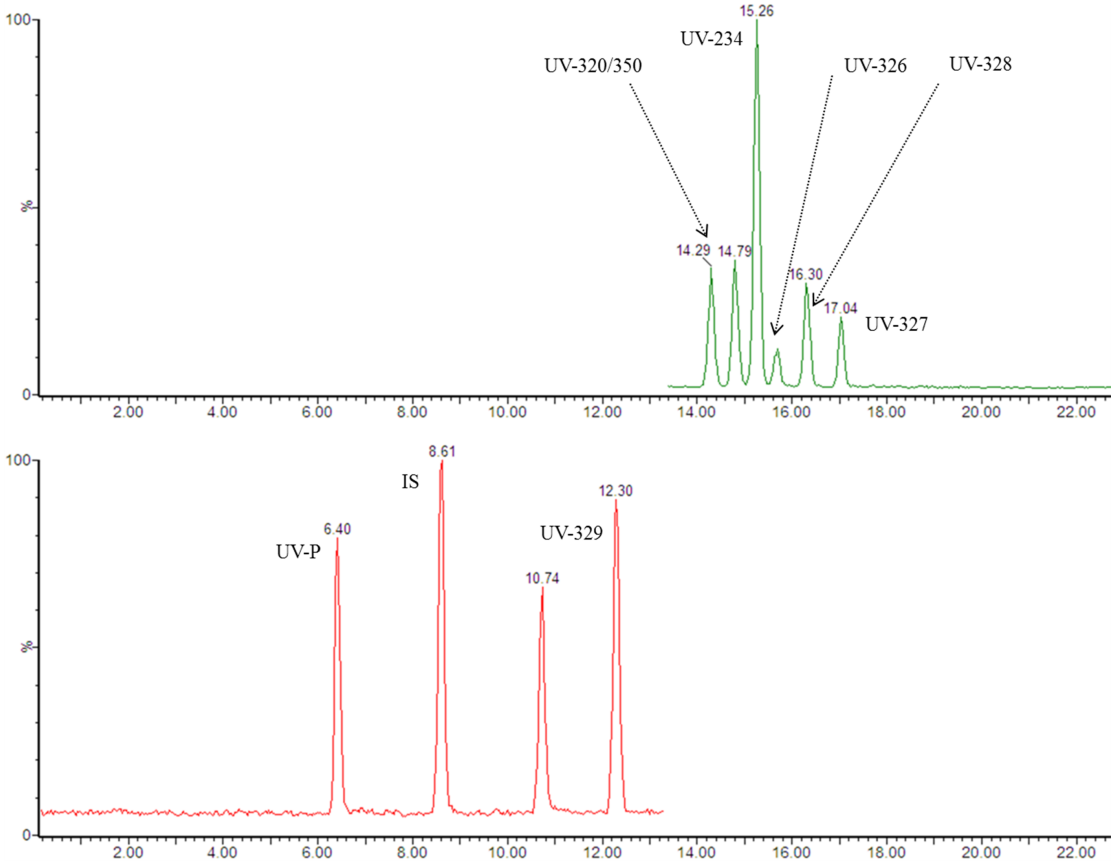

Figure S2 LC-MS/MS chromatograms of target BZT-UV analogues at concentration of 5 ng/g.