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

Supplementary Information

Pharmaceutical and anticorrosive substance removal by woodchip column reactor: removal process and effects of operational parameters

Yu-Jung Tseng [a], Webber Wei-Po Lai [a], Hsin-hsin Tung [a], Angela Yu-Chen Lin [a,b*]

[a] Graduate Institute of Environmental Engineering, National Taiwan University, 71-Chou-Shan Road, Taipei 106, Taiwan, ROC

[b] International Graduate Program of Molecular Science and Technology, National Taiwan University (NTU-MST), Taipei 106, Taiwan

(*corresponding author: yuchenlin@ntu.edu.tw; Tel: +886-2-3366-4386)

Contents

Table S1 Hydraulic properties of the experimental woodchip bioreactor columns.

column	woodchip type	drainable porosity [a]	specific retention [b]	total porosity [c]
Column_CA	Californian woodchips	0.5	0.34	0.84
Column_TW	Taiwanese woodchips	0.56	0.27	0.83

[a] drainable porosity: draining the columns from the bottom over a 1 h period.

[b] specific retention: measuring the difference between the wet woodchips that were removed from the column and dry woodchips that were dried in an oven at 50 °C for 48 hr.

[c] Total porosity: summation of drainable porosity and specific retention.

Text S1 LC−MS/MS analysis.

The sample injection volume was 20 μL. The autosampler was operated at room temperature. Quantifications were based on external standards. The detection limits for the seven target compounds were 1 μg/L. Multiple reaction monitoring transition (MRM) was applied to identified target compounds. Detailed LC−MS/MS information is provided in Tables S2 and S3.

Table S2 LC gradient conditions for (a) ACE, CAFF, CBZ, SFZ, BT, 5-MeBT and (b) IBU.

(a)

	ESI: positive mode		
Mobile phases	A: 0.1% formic acid in DI water B: 0.1% formic acid in MeOH		
Time (min)	Flow rate (μl/min)	Mobile A (%)	Mobile B (%)
0.0	1000	95	5
0.5	1000	95	5
2.0	1000	5	95
4.5	1000	5	95
5.0	1000	95	5
7.5	1000	95	5

(b)

	ESI: negative mode		
Mobile phases	A: 5 mM ammonium acetate in DI water B: 5 mM ammonium acetate in MeOH		
Time (min)	Flow rate (μl/min)	Mobile A (%)	Mobile B (%)
0.0	1000	90	10
0.5	1000	90	10
2.0	1000	10	90
4.5	1000	10	90
5.0	1000	90	10
7.0	1000	90	10

Table S3 Multiple reaction monitoring (MRM) mode experimental parameters.

Compound	Parent Ion (amu)	Product Ion (amu)	DP[a]	CE[a]	CXP[a]
ACE	152	93	32	32	4.1
		110	32	23.6	8.2
CAFF	195	110	35	30.4	8.3
		138	35	28.2	11
CBZ	237	192	43	29.1	15.6
		194	43	24.5	14
SFZ	256	92	40	36.5	4.4
		156	40	20	8
BT	120	92	50	24	6
		65	50	31	4
5-MeBT	134	106	50	24	8
		79	50	26	6
		77	50	36	5
IBU	205	161	−20	−9.7	−10.9

[a] DP: declustering potential; CE: collision energy; CXP: collision cell exit potential

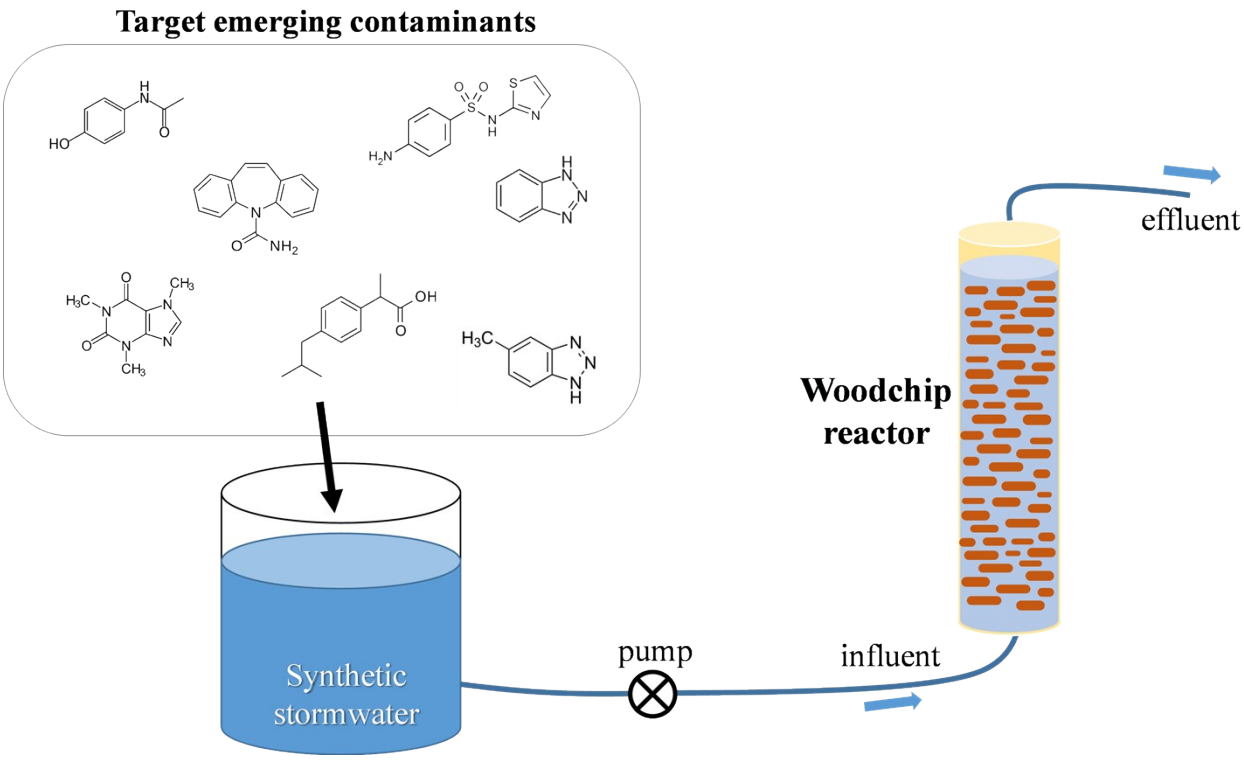

Figure S1 Schematic diagram of the woodchip column experimental setup.

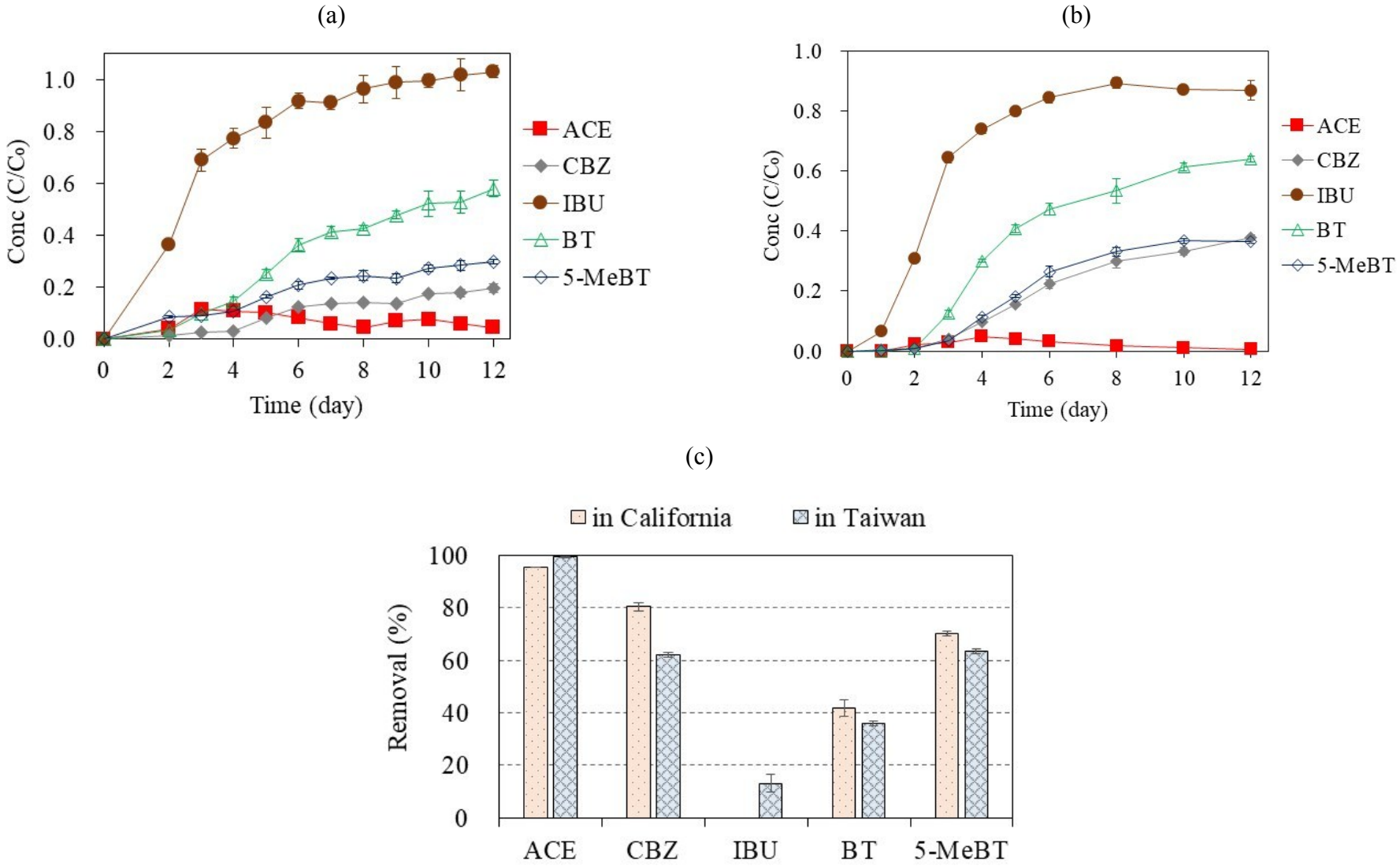

Figure S2 Target emerging contaminant removal in Column_CA in different regions: (a) in California, (b) in Taiwan and (c) removal (%) (condition: $[compound]_0$ = 1 mg/L; C/C_0 represents the effluent concentration of the target compound divided by the influent concentration (C_0)).

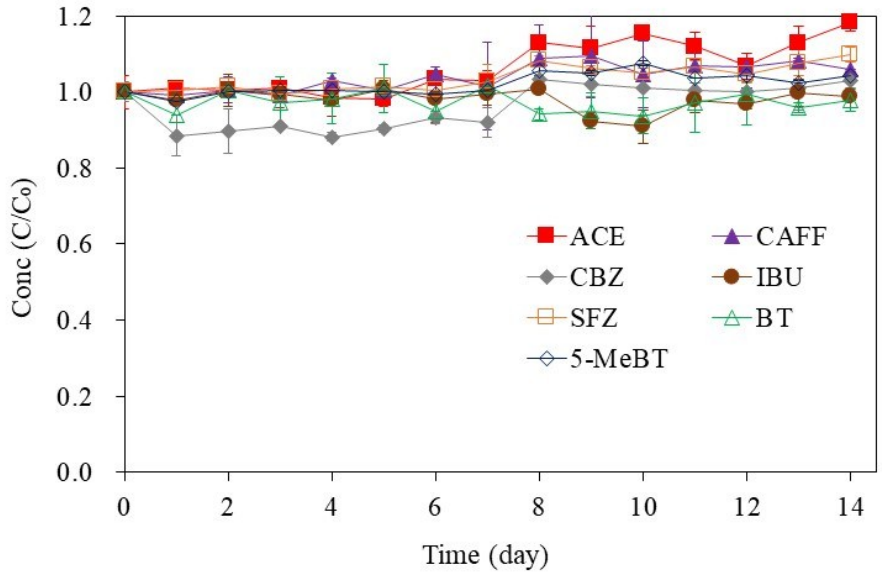

Figure S3 Hydrolysis test of the target compounds (condition: $[compound]_0$ = 100 µg/L).

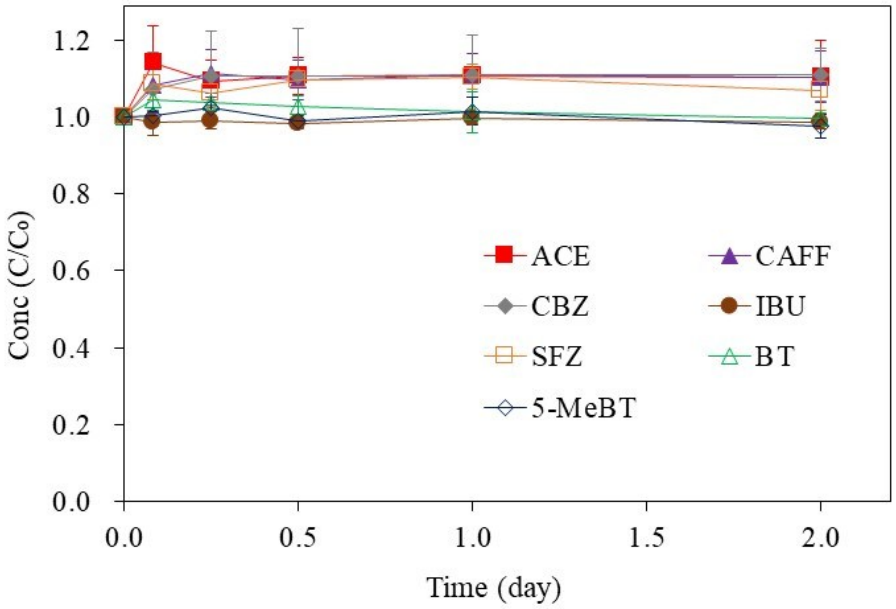

Figure S4 Sorption test of the target compounds by expanded clay (condition: $[compound]_0$ = 100 µg/L, expanded clay amount = 2 g, batch reactor volume = 100 mL; y axis shows the aqueous phase concentration of the target compounds).

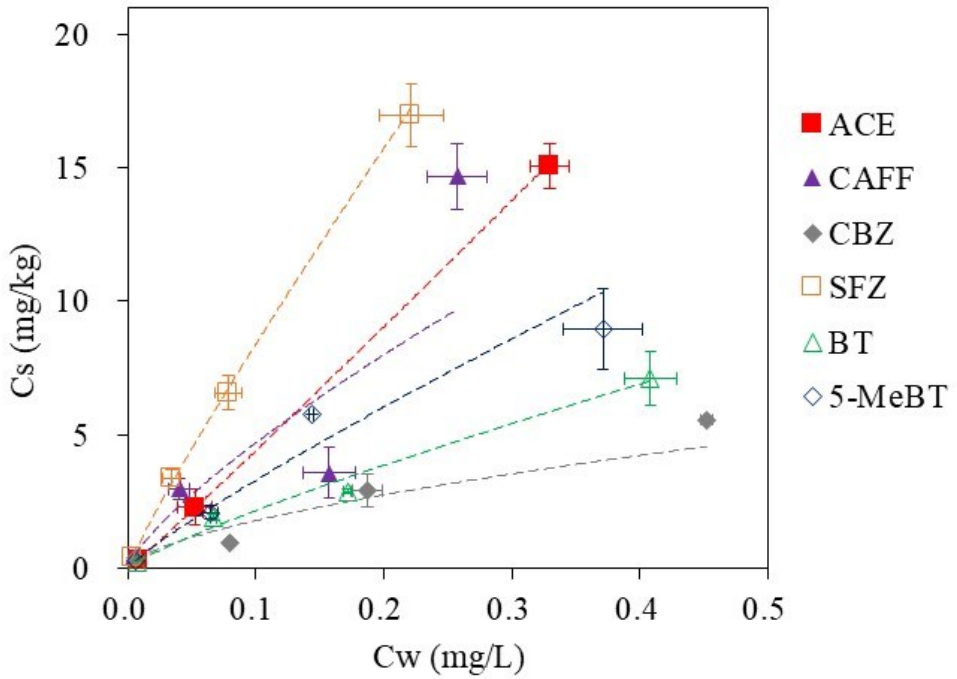

Figure S5 Freundlich sorption isotherms of target compounds with Californian woodchips.

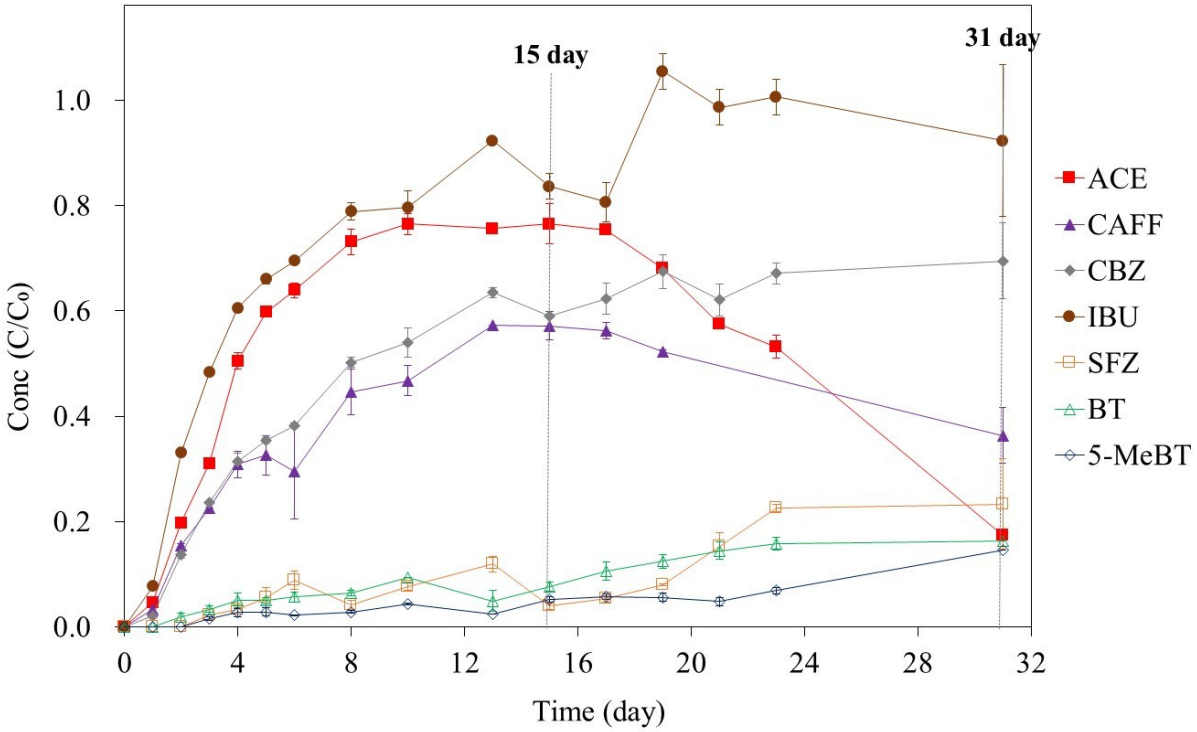

Figure S6 Effect of operation time on target emerging contaminant removal in Column_TW. (condition: $[compound]_0$ = 100 μg/L; C/C_0 represents the effluent concentration of the target compound divided by the influent concentration (C_0)).