Advancing Sequential Managed Aquifer Recharge Technology (SMART) Using Different Intermediate Oxidation Processes

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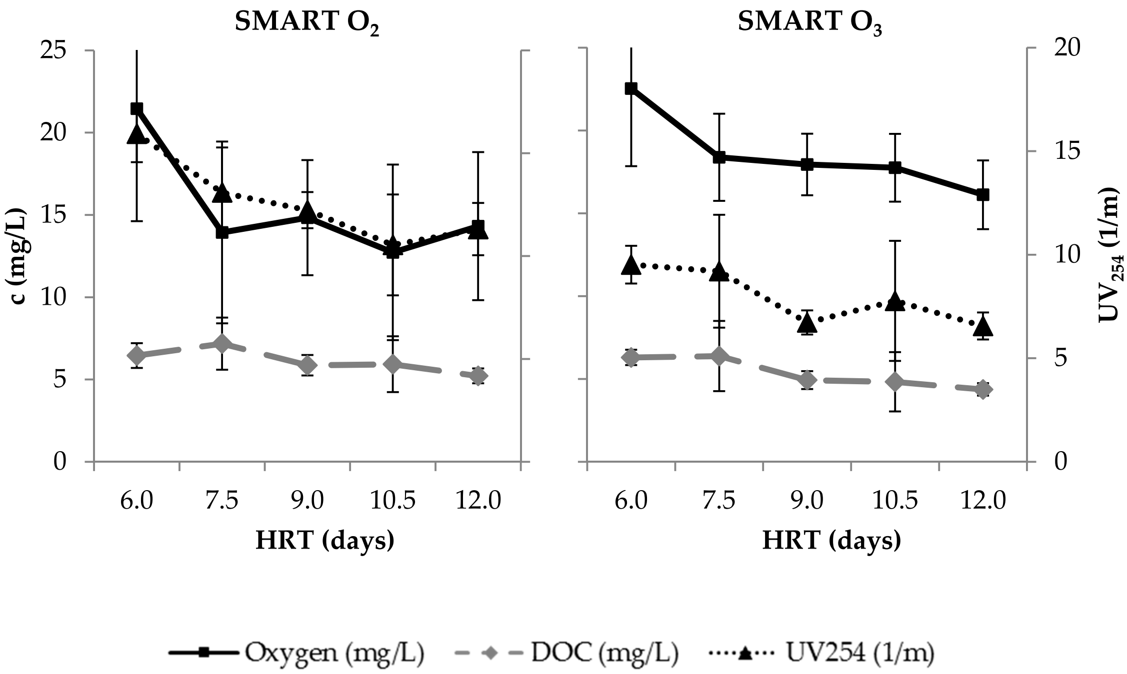

Figure S1. Profile data of the DO, DOC and UV_{254} measurements of the systems SMART O_2 and SMART O_3 after aeration with pure oxygen or ozone, respectively ($n \geq 4$).

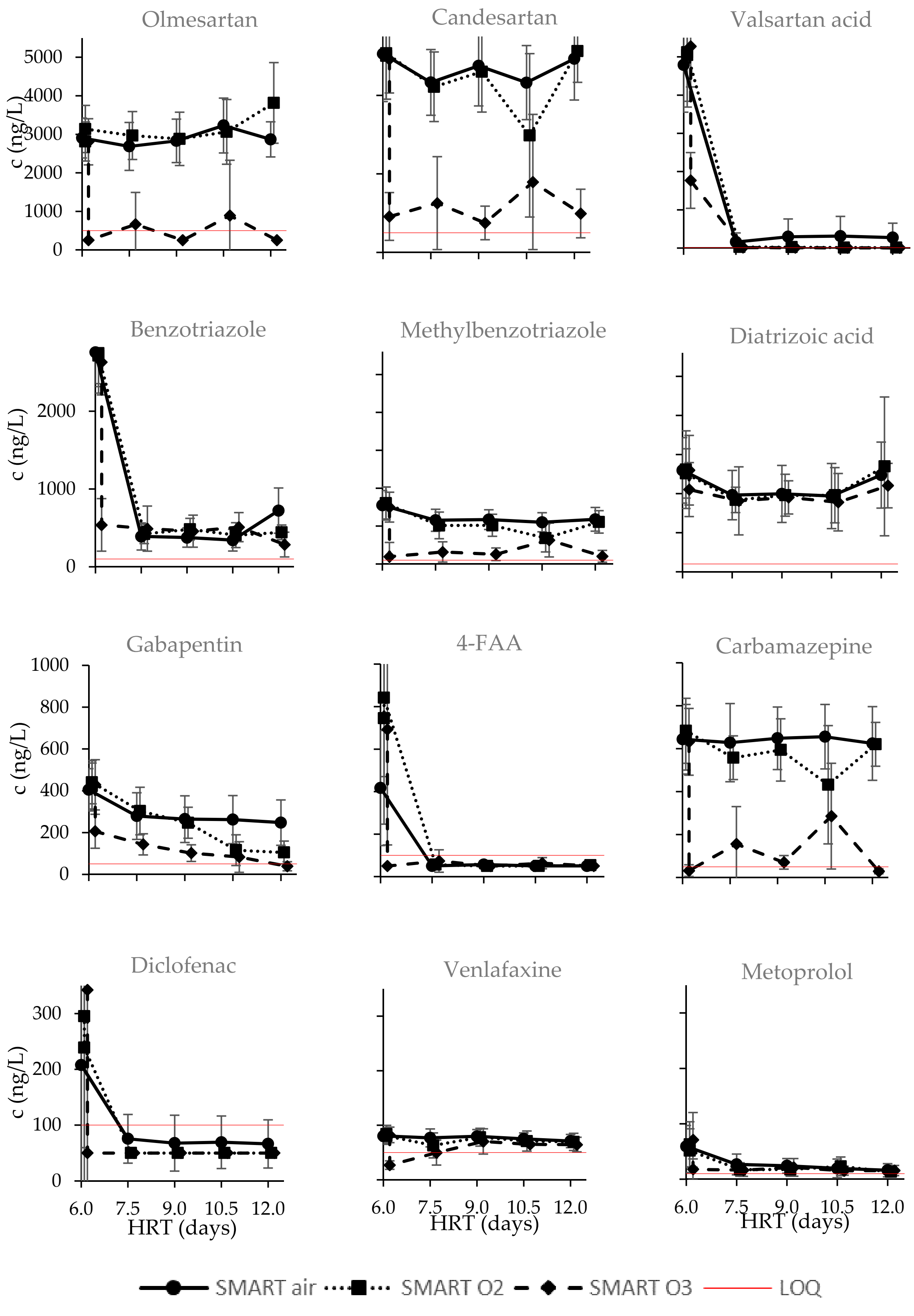

Figure S2. Profile data of the systems SMART air, SMART O_2 and SMART O_3 after aeration with air, pure oxygen or ozone, respectively, of all quantified TOrCs with effluent concentrations of the first filtration step > LOQ despite sulfamethoxazole. Values < LOQ are referred to LOQ/2.Results are shown as mean values with standard deviation as error bars (n ≥4).

Table S1. List of quantified TOrCs.

Compound	Molecular Formular	Influent Concentration (ng/L)	LOQ (ng/L)	k_{O3} ($M^{-1}s^{-1}$)	k_{OH} ($M^{-1}s^{-1}$)	Fragments Quantifier/Qualifier (m/z)	Internal Standard
Acesulfame	$C_4H_5NO_4S$	556 ± 276	250	88 [1]	4.6×10^9 [1]	82.1/78.0	acesulfame-d4_86.1 / acesulfame-d4_78.0
Benzotriazole	$C_6H_5N_3$	2603 ± 472	100	2.4×10^2 [2]	7.6×10^9 [3]	65.0/92.0	benzotriazole-d4_69.1/benzotriazole-d4_96.1
Candesartan	$C_{24}H_{20}N_6O_3$	5448 ± 1099	500	-	-	263/423	benzotriazole-d4_143.0/benzotriazole-d4_320.0
Carbamazepine	$C_{15}H_{12}N_2O$	667 ± 191	50	~ 3×10^5 [4] [a]	$8.8 \pm 1.2 \times 10^9$ [4] [b]	194.1/179.1	carbamazepine-d8_202.1/carbamazepine-d8_185.1
Diatrizoic acid *	$C_{11}H_9I_3N_2O_4$	1667 ± 911	100	0.05 ± 0.01 [5]	$5.4 \pm 0.3 \times 10^8$ [5]	361.0/233.0	iopromide-d3_575.8/iopromide-d3_299.6
Diclofenac	$C_{14}H_{11}Cl_2NO_2$	1291 ± 444	100	~ 1×10^6 [4] [a]	$7.5 \pm 1.5 \times 10^9$ [4] [b]	214.0/179.0	diclofenac-d4_218.0/diclofenac-d4_183.0
Gabapentin	$C_9H_{17}NO_2$	517 ± 125	50	2.2×10^2 [2]	9.1×10^9 [2]	137.1/154.1	gabapentin-d4_139.1/gabapentin-d4_158.1
Iomeprol	$C_{17}H_{22}I_3N_3O_8$	1179 ± 414	100	similar to iopromide **	$2.0 \pm 0.1 \times 10^9$ [6]	531.9/404.9	iomeprol-d3_534.9/iomeprol-d3_407.9
Iopromide	$C_{18}H_{24}I_3N_3O_8$	970 ± 489	10	< 0.8 [4] [a]	$3.3 \pm 0.6 \times 10^9$ [4] [b]	572.8/299.6	iopromide-d3_575.8/iopromide-d3_299.6
Methylbenzotriazole	$C_7H_7N_3$	955 ± 250	50	4.0–4.9×10^2 [7]	-	77.0/79.1	5-methylbenzotriazole-d6_81.0/ 5-methylbenzotriazole-d6_85.0
Metoprolol	$C_{15}H_{25}NO_3$	450 ± 280	10	$2.0 \pm 0.6 \times 10^3$ [8]	$7.3 \pm 0.2 \times 10^9$ [8]	116.1/159.0	sulfamethoxazole-d4_160.0/ sulfamethoxazole-d4_112.0
Olmesartan	$C_{24}H_{26}N_6O_3$	3010 ± 641	500	-	-	207/429	5-methylbenzotriazole-d6_81.0/ 5-methylbenzotriazole-d6_85.0
Sulfamethoxazole	$C_{10}H_{11}N_3O_3S$	137 ± 54	50	~2.5×10^6 [4] [a]	$5.5 \pm 0.7 \times 10^9$ [4] [b]	156.0/108.0	sulfamethoxazole-d4_160.0/ sulfamethoxazole-d4_112.0
Valsartan	$C_{24}H_{29}N_5O_3$	422 ± 534	100	38 [2]	~10^{10} [2]	291.0/235.0	bezafibrate-d4_143.0/bezafibrate-d4_320.0
Valsartan acid	$C_{14}H_{10}N_4O_2$	3103 ± 582	10	-	-	206/178	5-methylbenzotriazole-d6_81.0/ 5-methylbenzotriazole-d6_85.0
Venlafaxine	$C_{17}H_{27}NO_2$	234 ± 69	50	8.5×10^3 [2]	~10^{10} [2]	58.0/260.0	carbamazepine-d8_202.1/carbamazepine-d8_185.1
4-Formylaminoantipyrine	$C_{12}H_{13}N_3O_2$	1656 ± 924	100	6.5×10^4 [9]	-	77.0/56.1	sulfamethoxazole-d4_160.0/ sulfamethoxazole-d4_112.0

[1] pH = 7, T = 20 °C; [2] pH = 7, T = 22 ± 2 °C; [3] pH = 5.8; [4] [a] pH = 7, T = 20 °C; [4] [b] pH = 7, T = 25 °C; [5] T = 20 °C; [6] pH = 7.0 ± 0.1, T = 22 ± 1 °C; [7] pH = 7; [8] pH = 7, 20–22 °C; [9] pH = 7, 20 °C; * k_{O3} and k_{OH} refer to diatrizoate; ** both compounds have similar structures.

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