catalysts

SUPPLEMENTARY INFORMATION

Solar Photocatalytic Degradation of Sulfamethoxazole by TiO_2 Modified with Noble Metals

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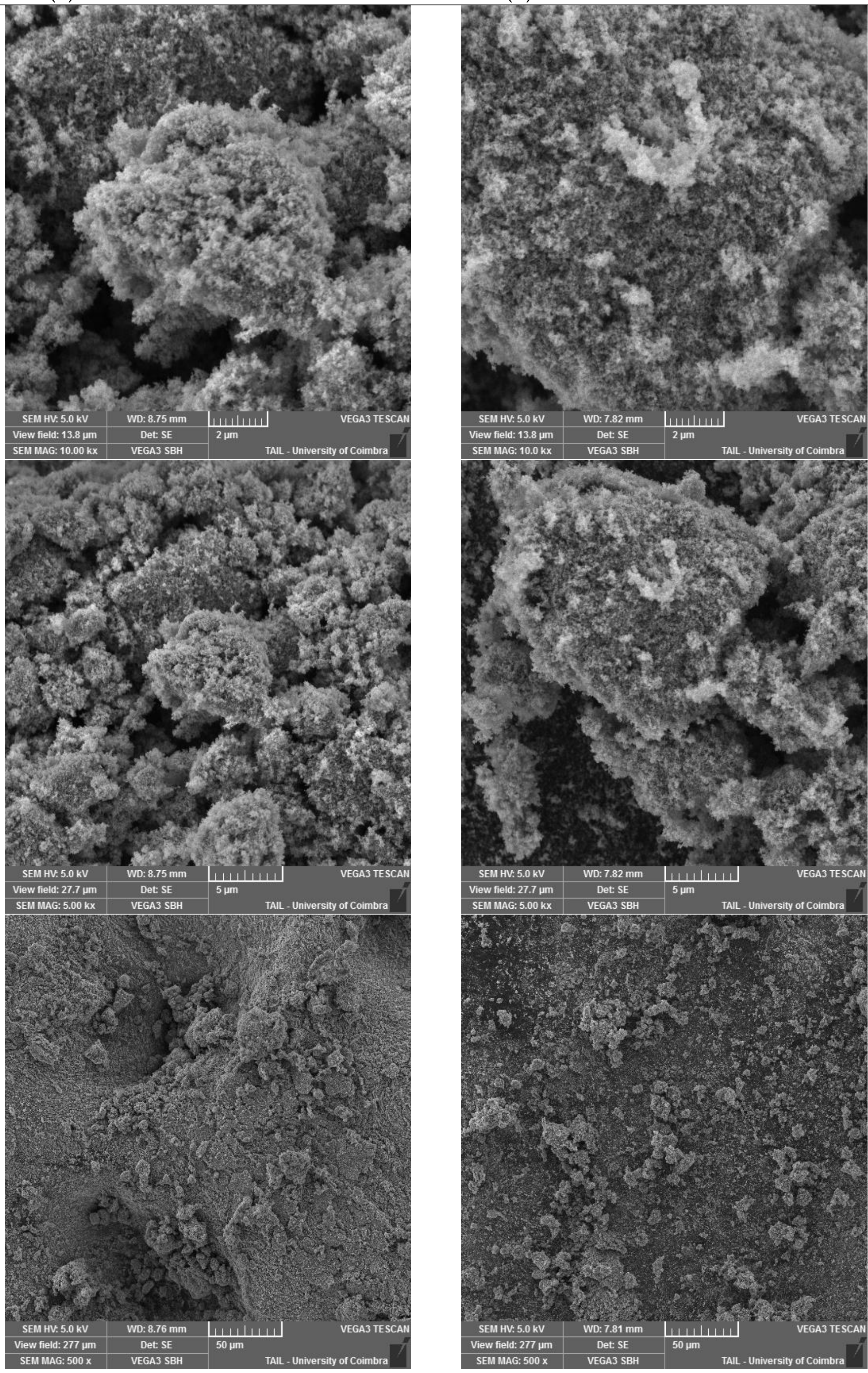
Magnitude (a) (b)

10'000 X

5'000 X

500 X



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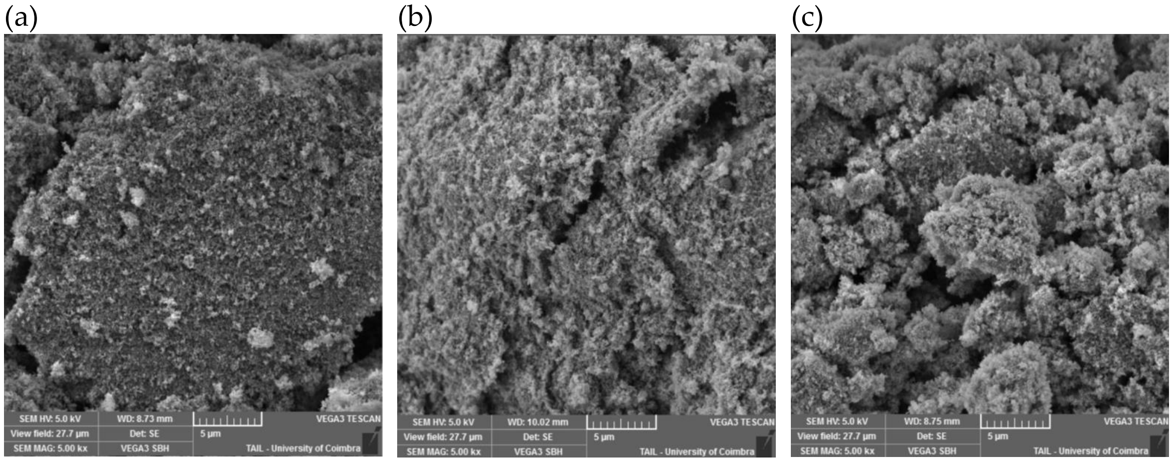

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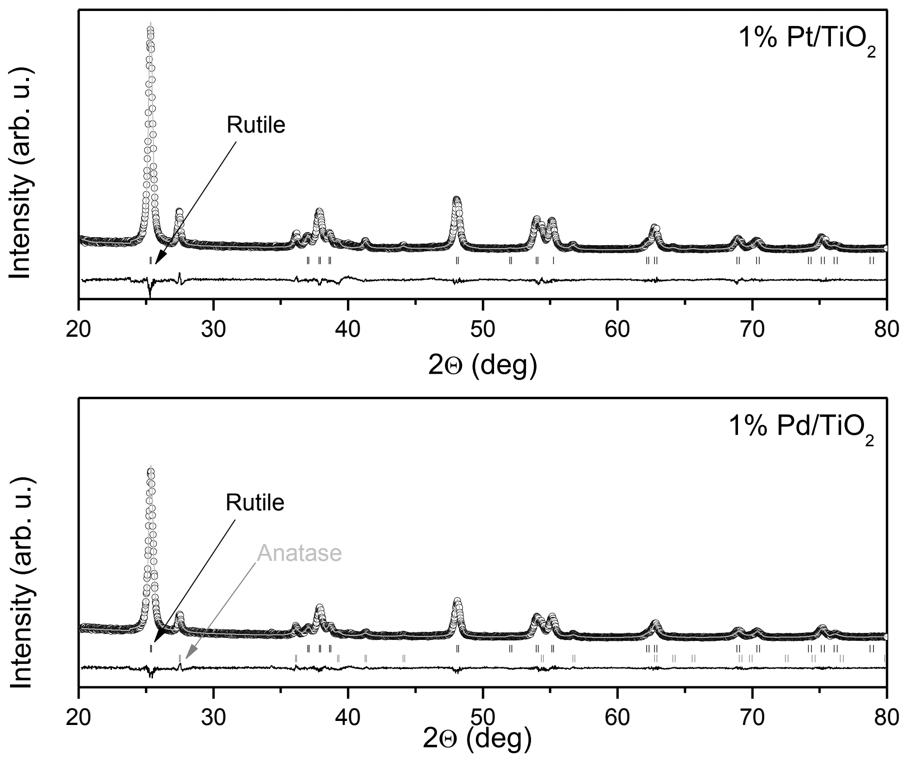
Table S1. XRD characterization of Pd/Pt-TiO_2 used in the study: distribution of anatase and rutile phases, unit cell parameters and crystallite size of photocatalysts particles.

	Anatase				Rutile			
	%	**a = b (Å)**	**c (Å)**	**Crystallite size (nm)**	**%**	**a = b (Å)**	**c (Å)**	**Crystallite size (nm)**
Pd (1%)	89	3.7842 (3)	9.5045 (9)	206	11	4.5927 (7)	2.9608 (6)	180
Pt (1%)	80	3.7832 (3)	9.5009 (7)	220	20	4.5910 (5)	2.9573 (7)	216



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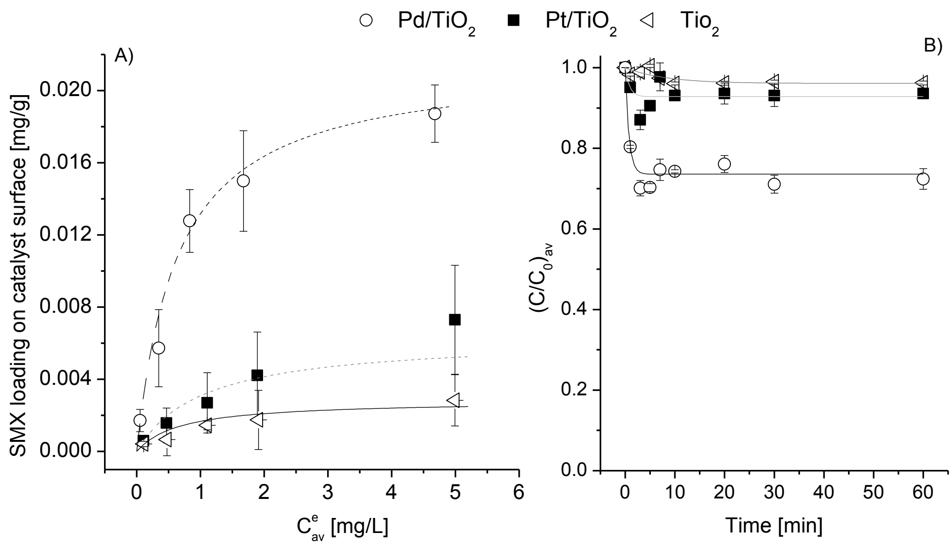

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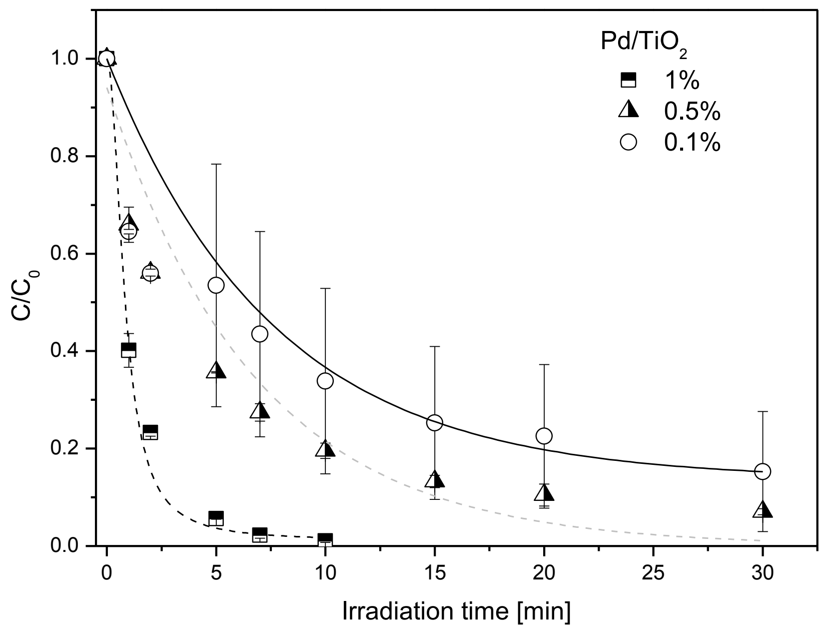
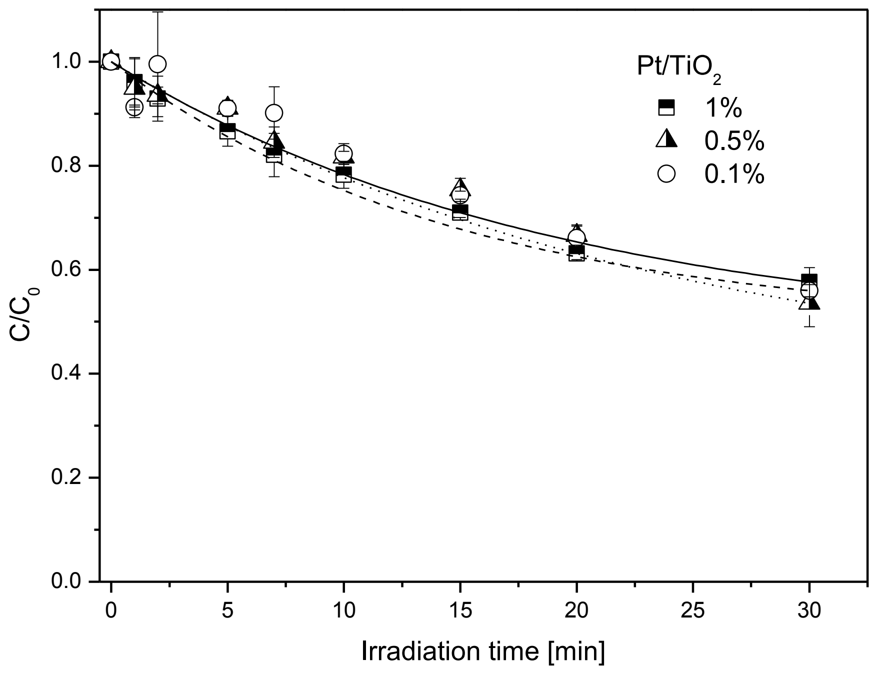


Figure S5. Solar photocatalytic degradation of sulfamethoxazole using Pd/TiO_2 (C_{cat}=~ 25 mg/L) at various modification levels.



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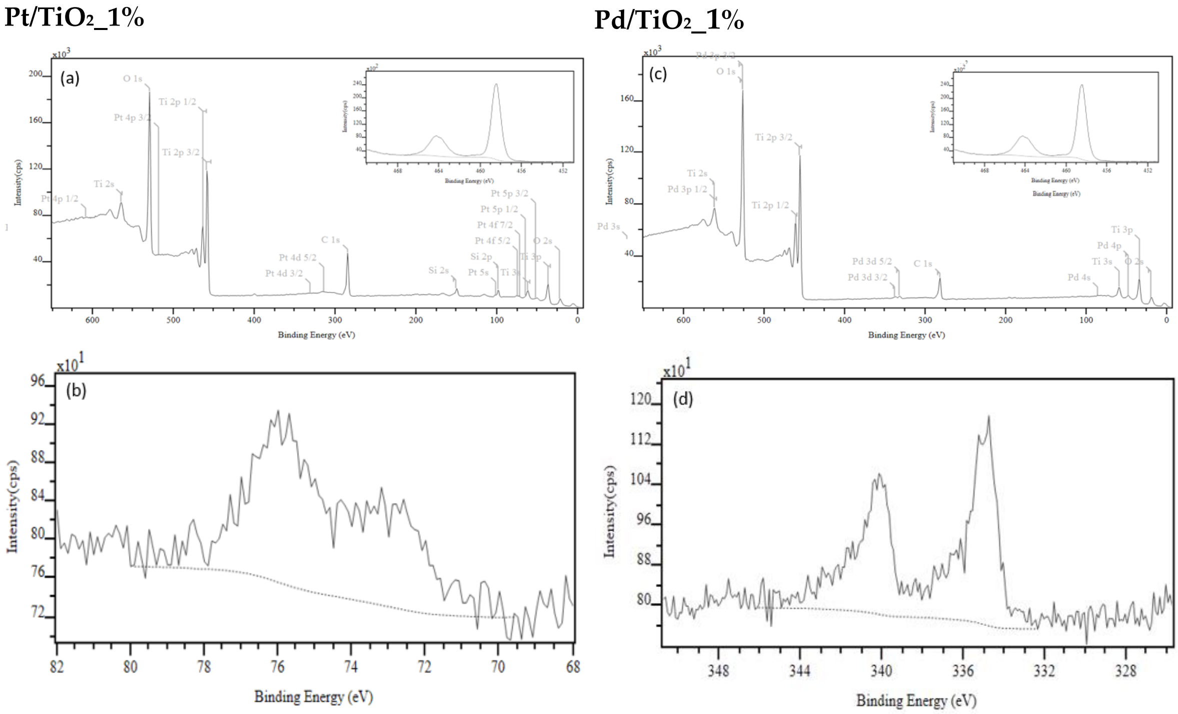

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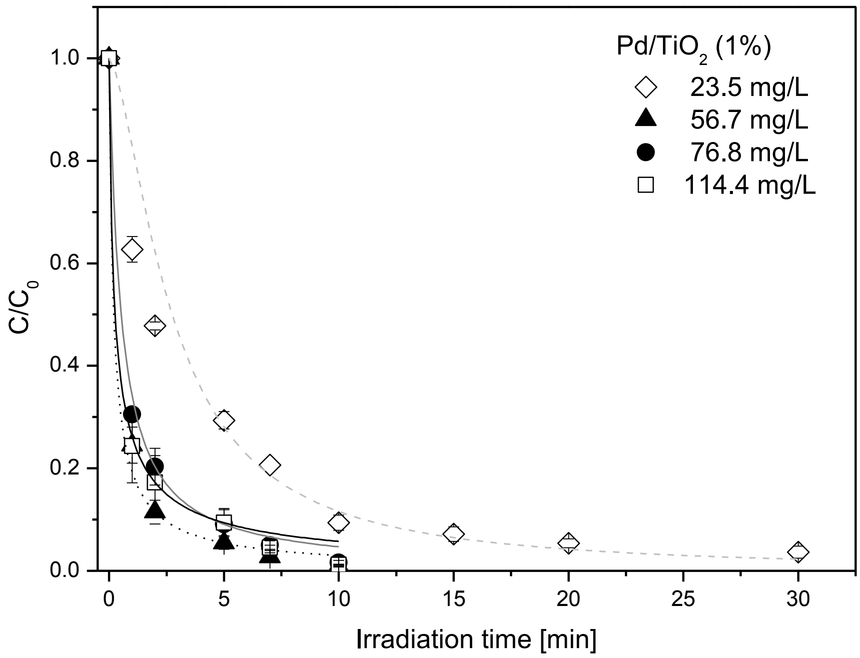


Figure S8. Solar photocatalytic degradation of sulfamethoxazole using Pd/TiO_2 (modification level 1%) at various initial concentration of catalysts.

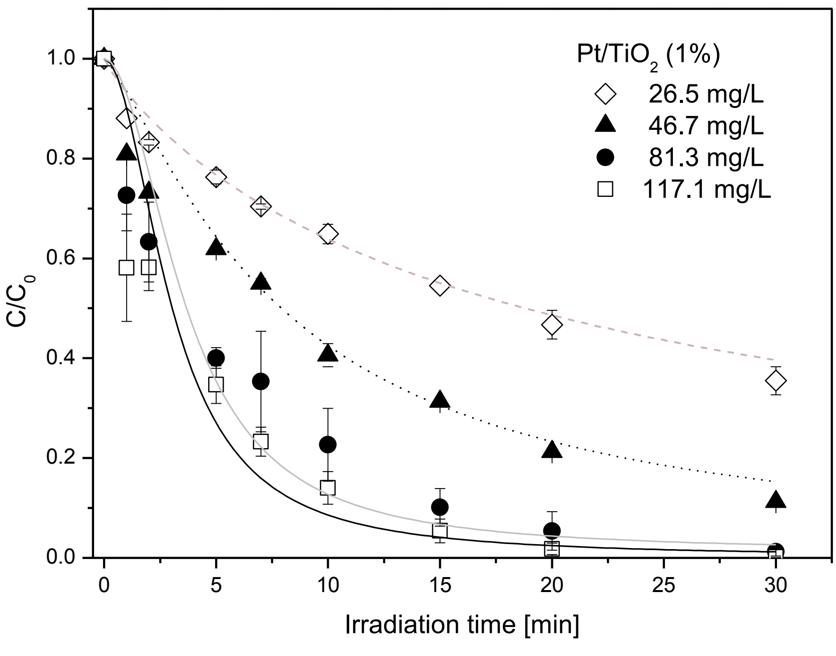


Figure S9. Solar photocatalytic degradation of sulfamethoxazole using Pt/TiO_2 (modification level 1%) at various initial concentration of catalysts.

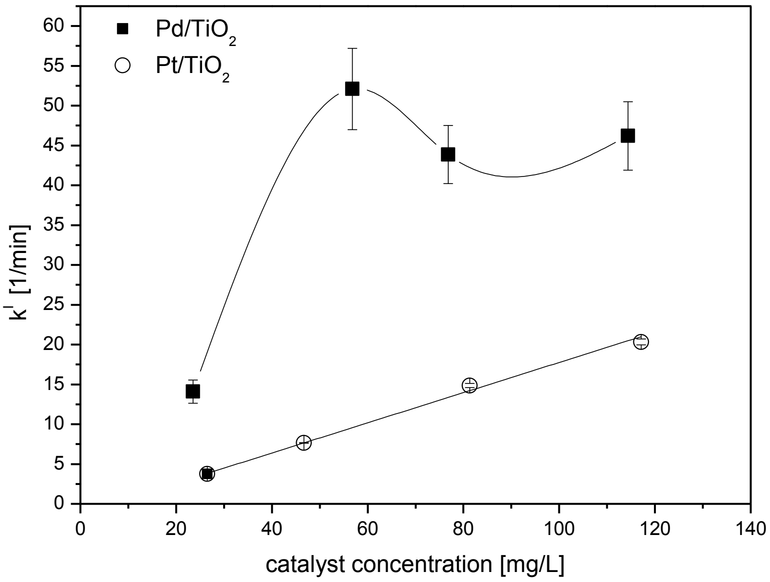


Figure S10. Dependence of pseudo-first order rate constant on the concentration of noble metal used for SMX photodegradation.

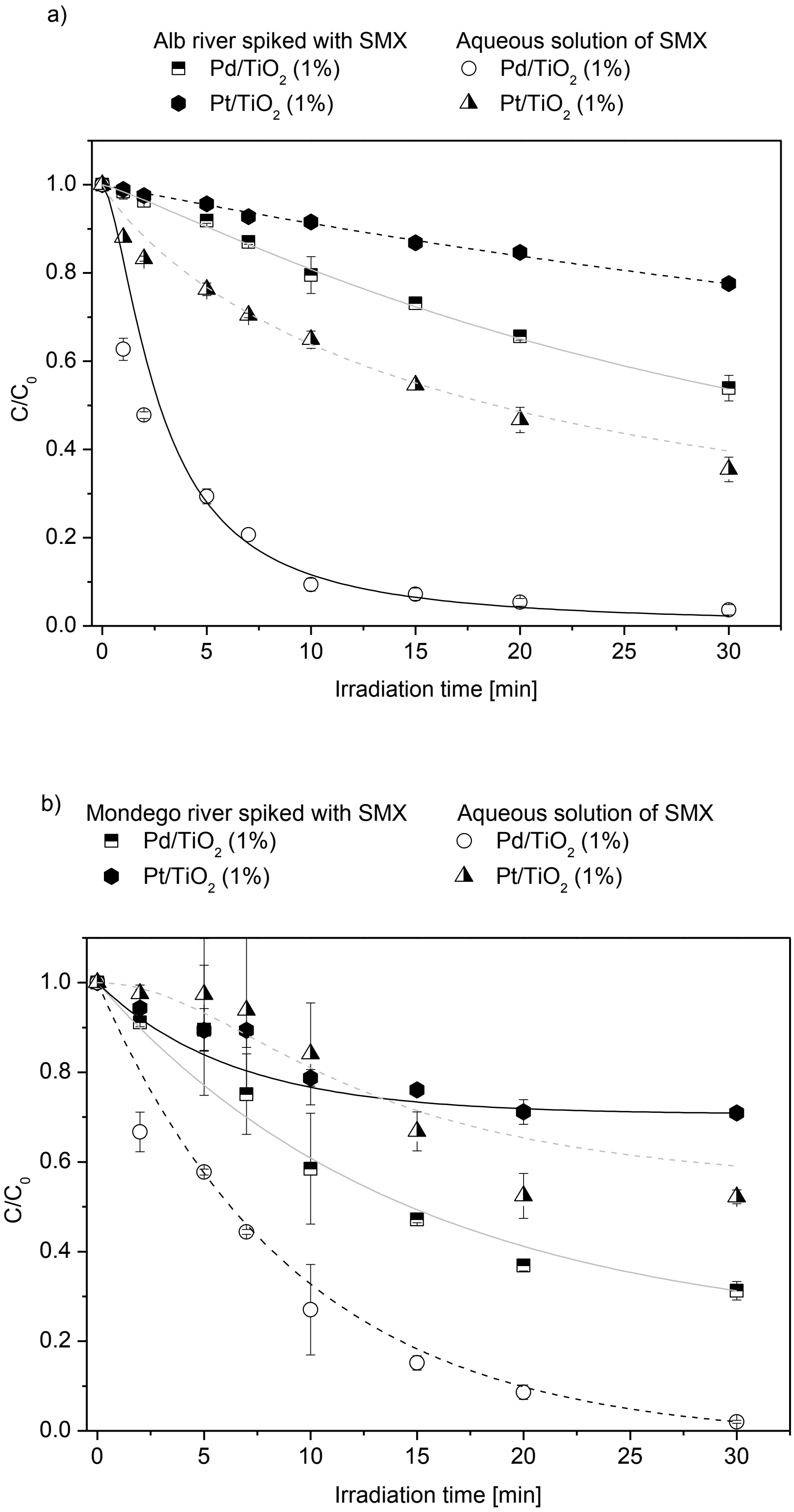
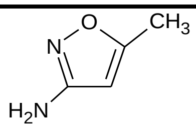
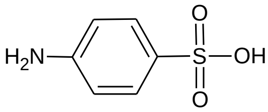
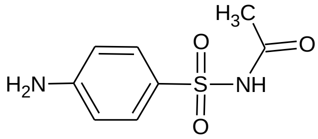
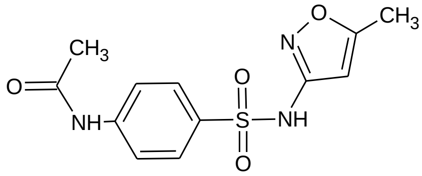
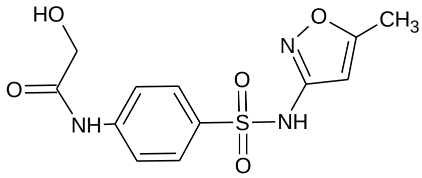
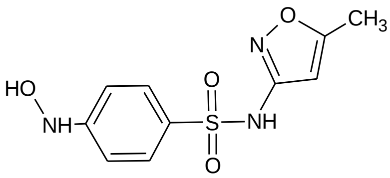
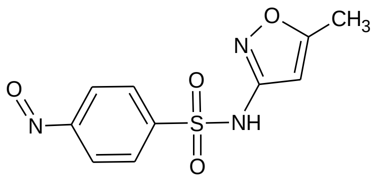
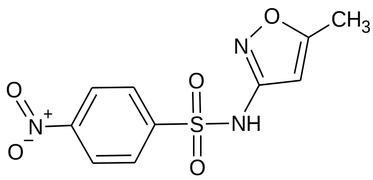
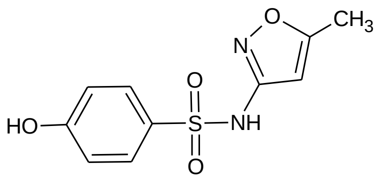
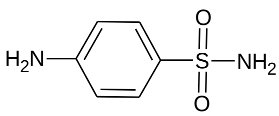


Figure S11. Comparison of solar photocatalytic degradation of sulfamethoxazole using Pt/TiO_2 and Pd/TiO_2 (modification level 1%, C_{cat}=~25 mg/L) in (a) Alb river water and (b) Mondego river water.

Table S2. Target analysis of TPs (based on [37])

Potential SMX TPs	Structure	Pd/TiO_2	Pt/TiO_2
3-Amino-5-methylisoxazol (3A5MI)		✓	✓
Sulfanilic acid (SA)		✗	✗
Sulfacetamid (SFAA)		(✓)	(✓)
Acetyl-sulfamethoxazole (Acetyl-SMX)		(✓)	(✓)
N-Hydroxy-acetyl-SMX (OH-acetyl-SMX)		(✓)	(✓)
N-Hydroxy-SMX (N-OH-SMX)		✓	✓
4-Nitroso-SMX (NO-SMX)		✓	✓
4-Nitro-SMX (NO_2-SMX)		✓	✓
4-Hydroxy-SMX (OH-SMX)		✗	✗
Sulfanilamid (SAD)		(✓)	(✓)

Brackets around the tick mean that the signals corresponding to the compound was detected, but due to the signal intensity, the formation of this compound is not certain.

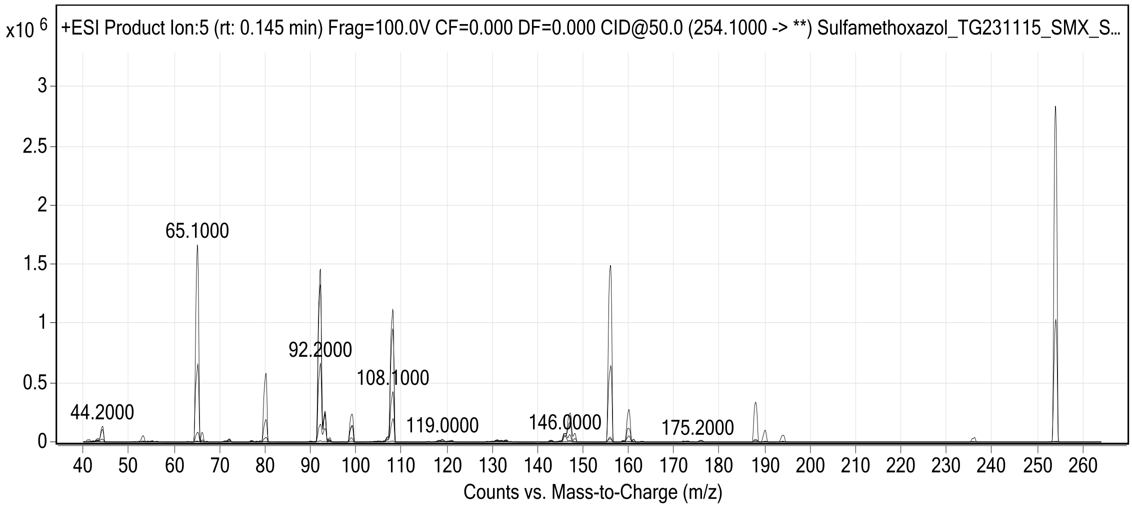


Figure S12. MS² spectrum of sulfamethoxazole (SMX). Precursor ion 254.0 m/z.

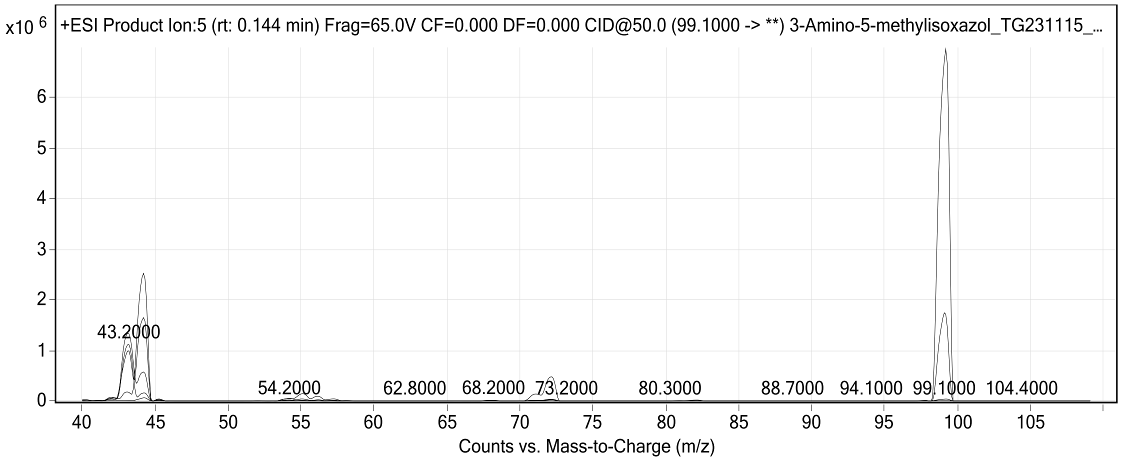


Figure S13. MS² spectrum of 3-amino-5-methylisoxazole (3A5MI). Precursor ion 99.1 m/z.

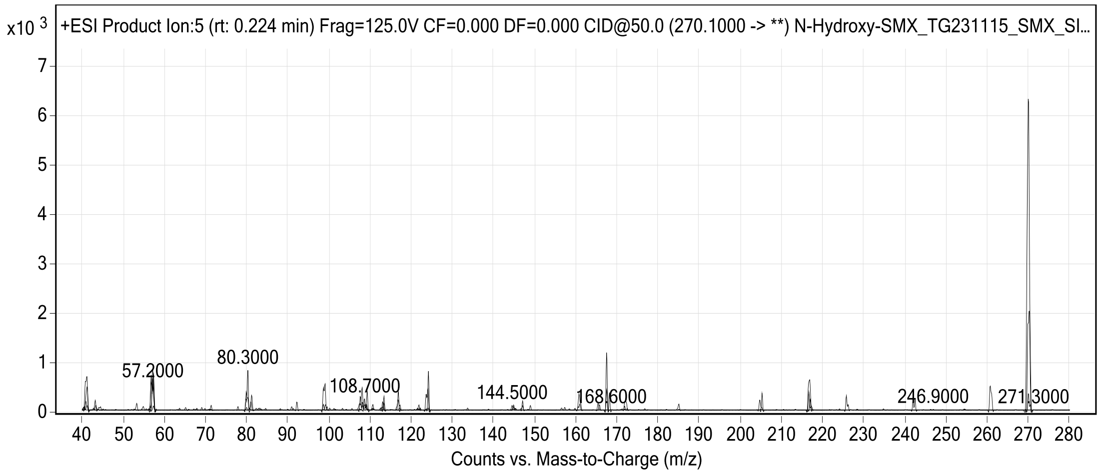


Figure S14. MS² spectrum of N-hydroxy-sulfamethoxazole (N-OH-SMX). Precursor ion 270.1 m/z.

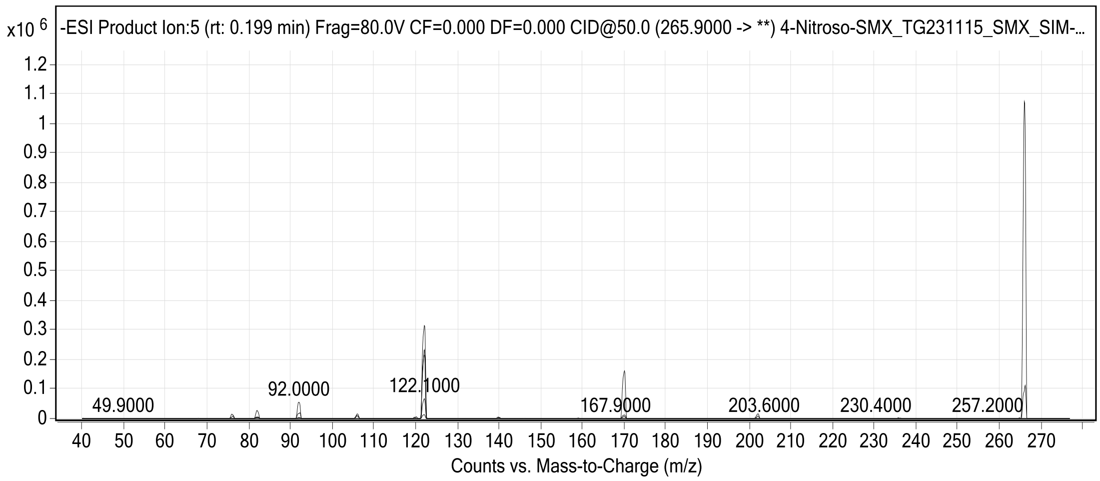


Figure S15. MS² spectrum of 4-nitroso -sulfamethoxazole (NO-SMX). Precursor ion 265.9 m/z.

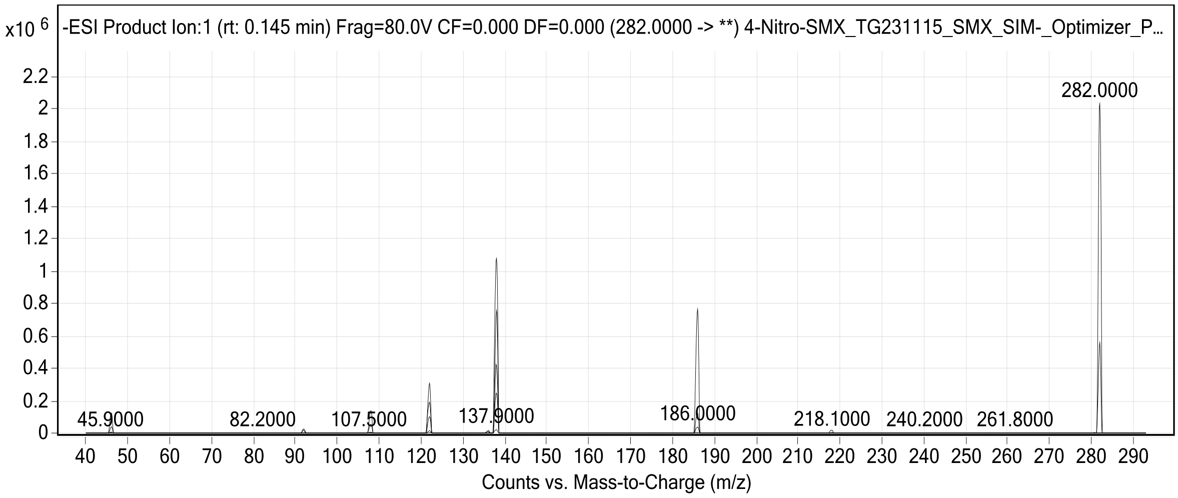
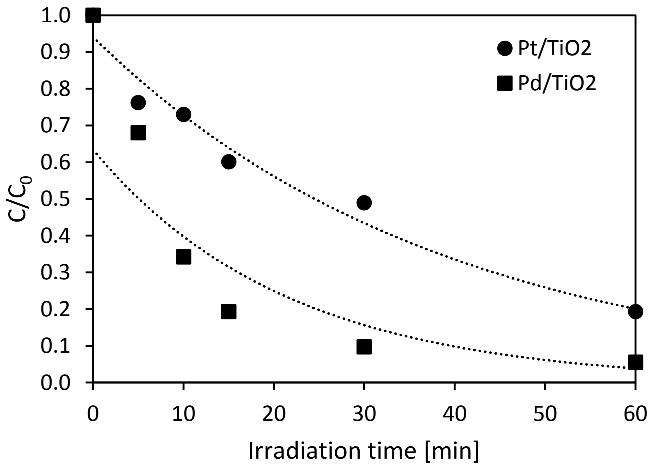


Figure S16. MS² spectrum of 4-nitro-sulfamethoxazole (NO2-SMX). Precursor ion 282.0m/z.



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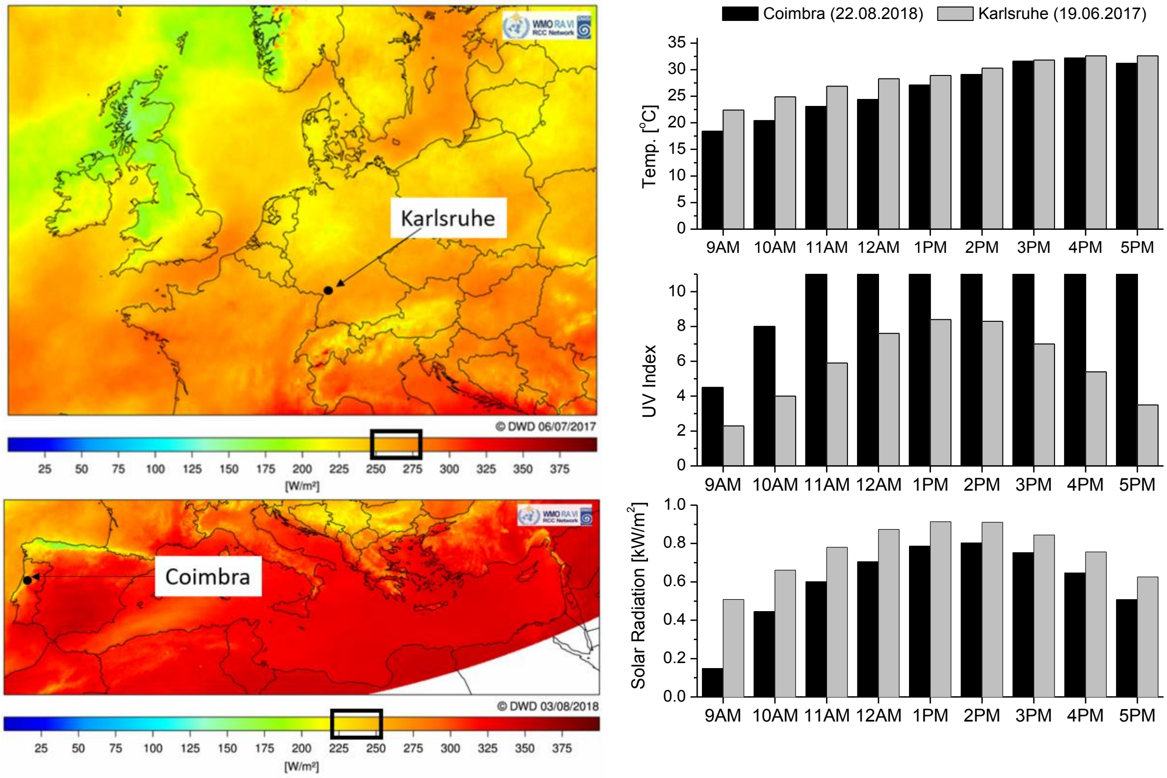

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Table S3. Physico-chemical parameters of Alb river water and Mondergo river water.

Parameter	Alb river	Mondego river
Total Organic Carbon (TOC)	5.5 mg/L	6.4 mg/L
Chemical Oxygen Demand (COD)	15.3 mgO_2/L	77 mgO_2/L
pH	7.4	6.3

Table S4. Settings of mass spectrometer source.

Source parameters	
Gas Temperature	200 ^{0}C
Gas Flow	8 L/min
Nebulizer	40 psi
Sheath Gas Temperature	300 ^{0}C
Sheath Gas Flow	12 L/min
Capillary	Positive: 4500 V
	Negative 3500 V
Nozzle Voltage	Positive 500 V
	Negative 300 V

Table S5. Optimized MS/MS parameters for determination of SMX and its TPs.

Compound	RT [min]	Polarity	Precursor Ion	Quantifier	CE [V]	Qualifier	CE [V]
SMX	4.5	Positive	254.1	155.9	12	92.0	28
SMX-d_4	4.5	Positive	258.1	156.0	36	151.1	12
3A5MI	1.2	Positive	99.1	72.1	10	55.1	10
SA	0.7	Negative	172.0	108	20	79.9	28
SFAA	1.6	Positive	214.9	92	26	65.1	42
Acetyl-SMX	5.0	Positive	296.0	197.8	10	133.9	22
OH-acetyl-SMX	4.3	Positive	312.0	149.9	22	77.1	50
N-OH-SMX	4.0	Positive	269.9	99.0	10	123.9	30
NO-SMX	7.7	Negative	265.9	121.9	22	169.9	10
NO_2-SMX	7.5	Negative	282.0	137.9	22	185.8	14
OH-SMX	5.0	Negative	252.9	146.9	10	93.0	26
SAD	0.7	Positive	172.8	128.8	14	117.0	10

RT- retention time, CE- collision energy