

Study of the phytoextraction and phytodegradation of sulfamethoxazole and trimethoprim from water by *Limnobium laevigatum*

Klaudia Stando^{1,*}, Aleksandra Czyż¹, Magdalena Gajda¹, Ewa Felis^{2,3},

Sylwia Bajkacz^{1,2}

¹ *Silesian University of Technology, Faculty of Chemistry, Department of Inorganic, Analytical Chemistry and Electrochemistry, B. Krzywoustego 6 Str., 44-100 Gliwice, Poland*

² *Silesian University of Technology, Biotechnology Centre, B. Krzywoustego 8 Str., 44-100 Gliwice, Poland*

³ *Silesian University of Technology, Faculty of Power and Environmental Engineering, Environmental Biotechnology Department, Akademicka 2 Str., 44-100 Gliwice, Poland*

SUPPLEMENTARY MATERIAL

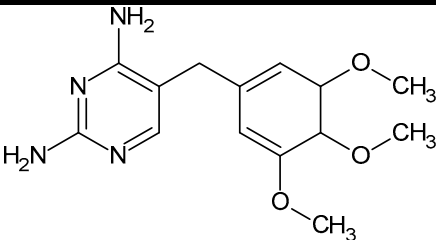
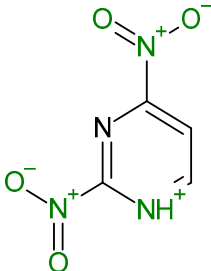
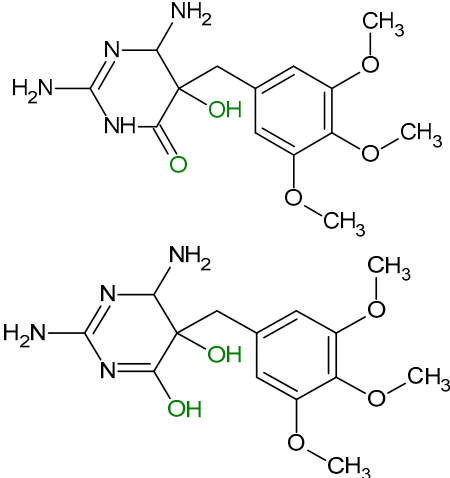
Summary

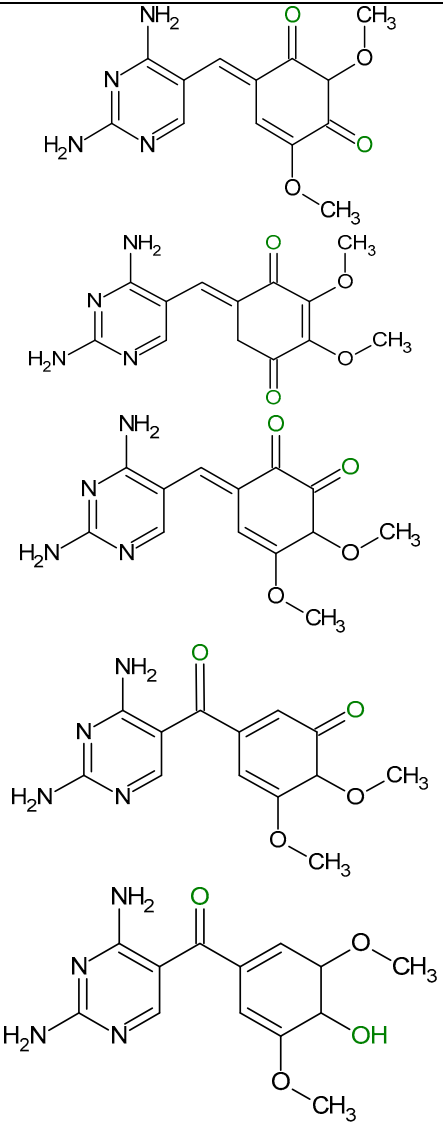
This supporting information file includes additional results and information as described in the text of the main article including:

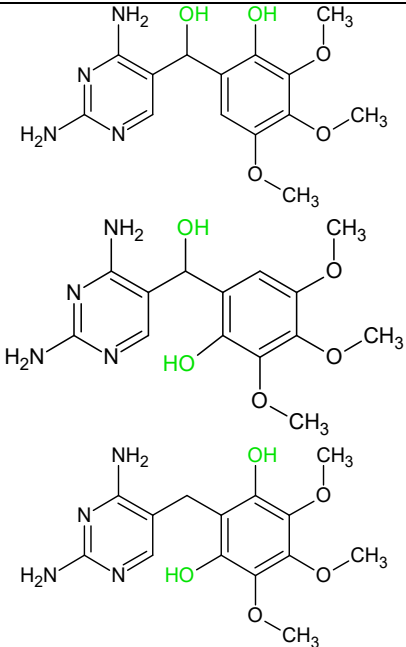
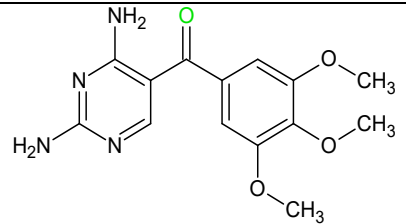
Table S1. Structures of identified SMX and TRI transformation products

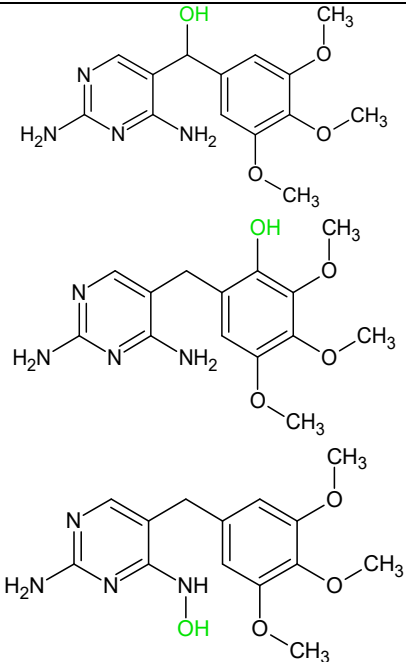
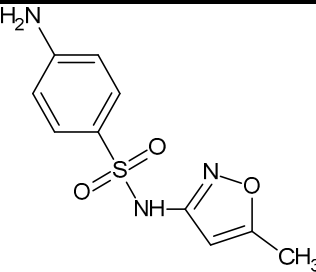
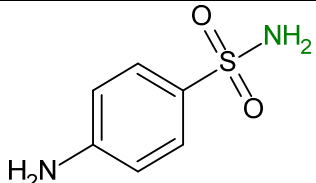
Figure S1. Representative LC-MS/MS chromatograms of the $[M+H]^+$ ions: TRI (m/z 291.2), (2) SMX (m/z 254.2)

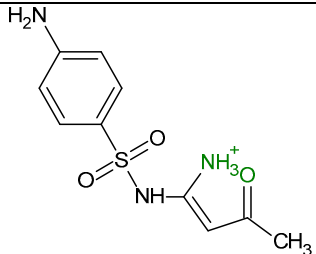
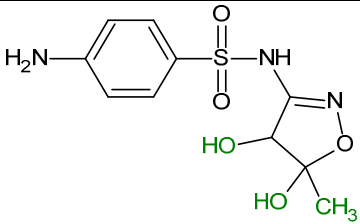
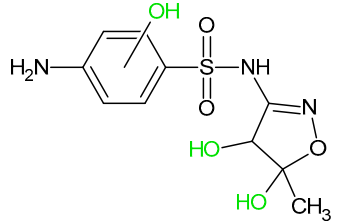
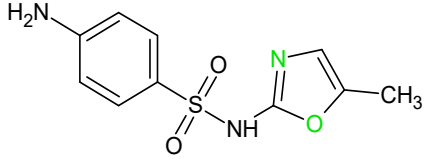
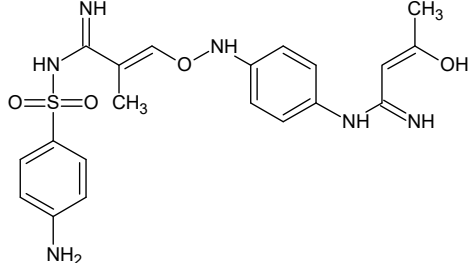
Table S1. Structures of identified SMX and TRI transformation products

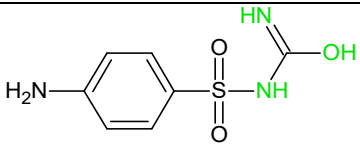
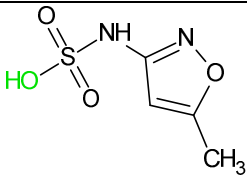
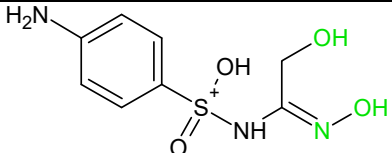
Abbreviation	Q ₁ (m/z)	Q ₃ (m/z)	Formula	Structure	Reference
TRI	291.2	123.1 230.1	C ₁₄ H ₁₈ N ₄ O ₃		-
TRI171	171.0	126.0 81.0	C ₄ H ₃ N ₄ O ₄ ⁺		[1]
TRI325	325.0	307.1 181.0	C ₁₄ H ₂₀ N ₄ O ₅		[2,3]

TRI291	291.1	258.1 261.2 231.1	$C_{13}H_{14}N_4O_4$		[2]
--------	-------	-------------------------	----------------------	--	-----

TRI323	323.1	231.1	C ₁₄ H ₁₈ N ₄ O ₅		[4]
TRI305	305.2	275.0	C ₁₄ H ₁₆ N ₄ O ₄		[5]

TRI307	307.1	259.1	C ₁₄ H ₁₈ N ₄ O ₄		[2]
SMX	254.2	108.1 156.0	C ₁₀ H ₁₁ N ₃ O ₃ S		-
SMX173	173.0	156.0 108.0 94.0	C ₆ H ₈ N ₂ O ₂ S		[6]

SMX256	256.1	214.1 173.0	C ₁₀ H ₁₄ N ₃ O ₃ S		[7]
SMX288	288.0	156.0 108.0 270.0	C ₁₀ H ₁₃ N ₃ O ₅ S		[6,8–10]
SMX304	304.1	286.9 275.0	C ₁₀ H ₁₀ N ₃ O ₆ S		This work
SMX254	254.0	156.0 108.0	C ₁₀ H ₁₁ N ₃ O ₃ S		[8]
SMX445	445.1	148.0 190.0	C ₂₀ H ₂₅ N ₆ O ₄ S		[7]

SMX216	216.0	156.0 92.0	C ₇ H ₉ O ₃ N ₃ S		[6]
SMX179	179.4	161.0 105.8	C ₄ H ₆ N ₂ O ₄ S		[8]
SMX246	246.0	156.0 92.0	C ₈ H ₁₂ N ₃ O ₄ S		[7]

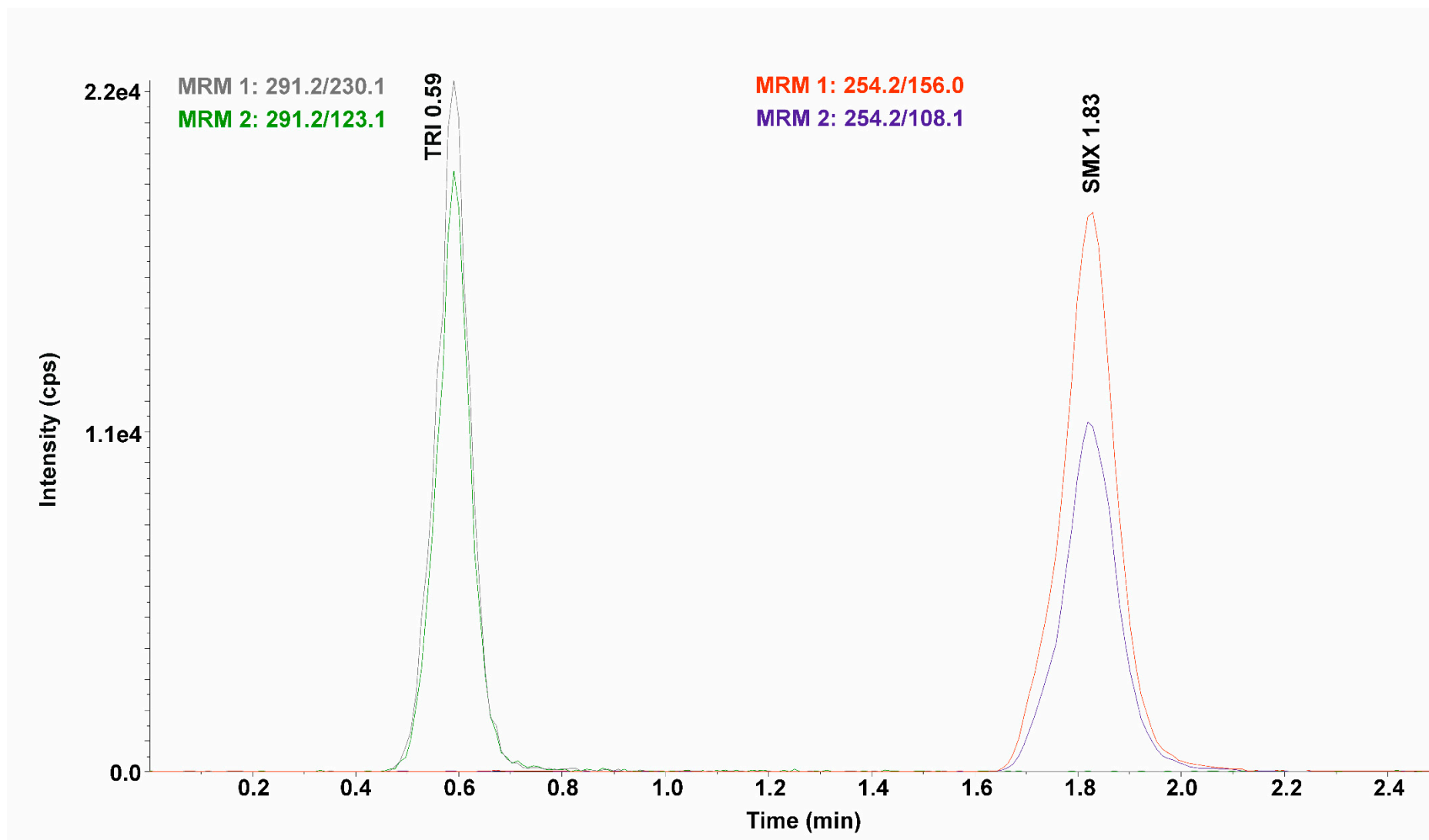


Figure S1. Representative LC-MS/MS chromatograms of the $[M+H]^+$ ions: TRI (m/z 291.2), (2) SMX (m/z 254.2)

References

1. Anquandah, G.A.K.; Sharma, V.K.; Knight, D.A.; Batchu, S.R.; Gardinali, P.R. Oxidation of Trimethoprim by Ferrate(VI): Kinetics, Products, and Antibacterial Activity. *Environ Sci Technol* **2011**, *45*, 10575–10581, doi:10.1021/es202237g.
2. Lecours, M.-A.; Eysseric, E.; Yargeau, V.; Lessard, J.; Brisard, G.; Segura, P. Electrochemistry-High Resolution Mass Spectrometry to Study Oxidation Products of Trimethoprim. *Environments* **2018**, *5*, 18, doi:10.3390/environments5010018.
3. Eichhorn, P.; Ferguson, P.L.; Pérez, S.; Aga, D.S. Application of Ion Trap-MS with H/D Exchange and QqTOF-MS in the Identification of Microbial Degradates of Trimethoprim in Nitrifying Activated Sludge. *Anal Chem* **2005**, *77*, 4176–4184, doi:10.1021/ac050141p.
4. Ji, Y.; Xie, W.; Fan, Y.; Shi, Y.; Kong, D.; Lu, J. Degradation of Trimethoprim by Thermo-Activated Persulfate Oxidation: Reaction Kinetics and Transformation Mechanisms. *Chemical Engineering Journal* **2016**, *286*, 16–24, doi:10.1016/j.cej.2015.10.050.
5. Alharbi, S.K.; Kang, J.; Nghiem, L.D.; van de Merwe, J.P.; Leusch, F.D.L.; Price, W.E. Photolysis and UV/H₂O₂ of Diclofenac, Sulfamethoxazole, Carbamazepine, and Trimethoprim: Identification of Their Major Degradation Products by ESI–LC–MS and Assessment of the Toxicity of Reaction Mixtures. *Process Safety and Environmental Protection* **2017**, *112*, 222–234, doi:10.1016/j.psep.2017.07.015.
6. Jia, Y.; Khanal, S.K.; Zhang, H.; Chen, G.H.; Lu, H. Sulfamethoxazole Degradation in Anaerobic Sulfate-Reducing Bacteria Sludge System. *Water Res* **2017**, *119*, 12–20, doi:10.1016/j.watres.2017.04.040.
7. Zheng, L.; Jin, H.; Yu, M.; Zhongwei, Q.; Zhang, L.; Shikun, C.; Li, Z. Degradation of Sulfamethoxazole by Electrochemically Activated Persulfate Using Iron Anode. *International Journal of Chemical Reactor Engineering* **2019**, *17*, 1–14, doi:10.1515/ijcre-2018-0160.
8. Gao, S.; Zhao, Z.; Xu, Y.; Tian, J.; Qi, H.; Lin, W.; Cui, F. Oxidation of Sulfamethoxazole (SMX) by Chlorine, Ozone and Permanganate-A Comparative Study. *J Hazard Mater* **2014**, *274*, 258–269, doi:10.1016/j.jhazmat.2014.04.024.

9. Kim, H.Y.; Kim, T.H.; Cha, S.M.; Yu, S. Degradation of Sulfamethoxazole by Ionizing Radiation: Identification and Characterization of Radiolytic Products. *Chemical Engineering Journal* **2017**, *313*, 556–566, doi:10.1016/j.cej.2016.12.080.
10. Gómez-Ramos, M. del M.; Mezcua, M.; Agüera, A.; Fernández-Alba, A.R.; Gonzalo, S.; Rodríguez, A.; Rosal, R. Chemical and Toxicological Evolution of the Antibiotic Sulfamethoxazole under Ozone Treatment in Water Solution. *J Hazard Mater* **2011**, *192*, 18–25, doi:10.1016/j.jhazmat.2011.04.072.