Peer-Reviewed Scientific Articles

de Carvalho, C.F.M., Lehmann, M.F., **Pati, S.G.** Variability in oxygen isotopic fractionation of enzymatic O_2 consumption. *Biogeosciences*, **2025**, 22, 4579-4600.

Pati, S.G., Brunner, L.M., Ley, M., Hofstetter, T.B. Oxygen isotope fractionation of O_2 consumption through abiotic photochemical singlet oxygen formation pathways. *ACS Environmental Au*, **2025**, 5, 220-229.

Hofstetter, T.B., Bakkour, R., Buchner, D., Eisenmann, H., Fischer, A., Gehre, M., Haderlein, S.B., Höhener, P., Hunkeler, D., Imfeld, G., Jochmann, M.A., Kümmel, S., Martin, P.R., **Pati, S.G.**, Schmidt, T.C., Vogt, C., Elsner, M., Perspectives of compound-specific isotope analysis of organic contaminants for assessing environmental fate and managing chemical pollution. *Nature Water*, **2024**, 2, 14-30.

de Carvalho, C.F.M., Lehmann, M.F., **Pati, S.G.** Improving the accuracy of $\delta^{18}O$ and $\delta^{17}O$ values of O_2 measured by continuous-flow isotope-ratio mass spectrometry with a multipoint isotope-ratio calibration. *Rapid Communications in Mass Spectrometry*, **2024**, 38, e9652.

Bopp, C.E., Bolotin, J., **Pati, S.G.**, Hofstetter, T.B. Managing argon interference during measurements of $^{18}O/^{16}O$ ratios in O_2 by continuous-flow isotope ratio mass spectrometry. *Analytical and Bioanalytical Chemistry*, **2022**, 414, 6177-6186.

Pati, S.G., Bopp, C.E., Kohler, H.-P.E., Hofstetter, T.B. Substrate-specific coupling of O_2 activation to hydroxylations of aromatic compounds by Rieske non-heme iron dioxygenases. *ACS Catalysis*, **2022**, 12, 6444-6456.

Hora, P.I., **Pati, S.G.**, McNamara, P.J., Arnold, W.A. Increased use of quaternary ammonium compounds during the SARS-CoV-2 pandemic and beyond: Consideration of environmental implications. *Environmental Science and Technology Letters*, **2020**, 7, 622-631.

Pati, S.G., Arnold, W.A. Comprehensive screening of quaternary ammonium surfactants and ionic liquids in wastewater effluents and lake sediments. *Environmental Science: Processes & Impacts*, **2020**, 22, 430-441.

Pati, S.G., Arnold, W.A. Reaction rates and product formation during advanced oxidation of ionic liquid cations by UV/peroxide, UV/persulfate, and UV/chlorine. *Environmental Science: Water Research and Technology*, **2018**, 4, 1310-1320.

Pati, S.G., Arnold, W.A. Photochemical transformation of four ionic liquid cation structures in aqueous solution. *Environmental Science and Technology*, **2017**, 51, 11780-11787.

Maier, M.P., Prasse, C., **Pati, S.G.**, Nitsche, S., Zhe, L., Radke, M., Meyer, A., Hofstetter, T.B., Ternes, T.A., Elsner, M. Exploring trends of C and N isotope fractionation to trace transformation reactions of diclofenac in natural and engineered systems. *Environmental Science and Technology*, **2016**, 50, 10933-10942.

Pati, S.G., Kohler, H.-P.E., Pabis, A., Paneth, P., Parales, R.E., Hofstetter, T.B. Substrate and enzyme specificity of the kinetic isotope effects associated with the dioxygenation of nitroaromatic contaminants. *Environmental Science and Technology*, **2016**, 50, 6708-6716.

Pati, S.G., Bolotin, J., Brennwald, M.S., Kohler, H.-P.E., Werner, R.A., Hofstetter, T.B. Measurement of oxygen isotope ratios ($^{18}O/^{16}O$) of aqueous O_2 in small samples by gas chromatography/isotope ratio mass spectrometry. *Rapid Communications in Mass Spectrometry*, **2016**, 30, 684-690.

Wijker, R.S., **Pati, S.G.**, Zeyer, J., Hofstetter, T.B. Enzyme kinetics of different types of flavin-dependent monooxygenases determine the observable contaminant stable isotope fractionation. *Environmental Science and Technology Letters*, **2015**, 2, 329-334.

Hofstetter, T.B., Bolotin, J., **Pati, S.G.**, Skarpeli-Liati, M., Spahr, S., Wijker, R.S. Isotope effects as new proxies for organic pollutant transformation. *CHIMIA*, **2014**, 68, 788-792.

Pati, S.G., Kohler, H.-P.E., Bolotin, J., Parales, R.E., Hofstetter, T.B. Isotope effects of enzymatic dioxygenation of nitrobenzene and 2-nitrotoluene by nitrobenzene dioxygenase. *Environmental Science and Technology*, **2014**, 48, 10750-10759.

Pati, S.G., Shin, K., Skarpeli-Liati, M., Bolotin, J., Eustis, S.N., Spain, J.C., Hofstetter, T.B. Carbon and nitrogen isotope effects associated with the dioxygenation of aniline and diphenylamine. *Environmental Science and Technology*, **2012**, 46, 11844-11853.

Skarpeli-Liati, M., **Pati, S.G.**, Bolotin, J., Eustis, S.N., Hofstetter, T.B. Carbon, hydrogen, and nitrogen isotope fractionation associated with oxidative transformation of substituted aromatic *N*-alkyl amines. *Environmental Science and Technology*, **2012**, 46, 7189-7198.

E-book Series Chapters

Bopp, C.E., Bernet, N.M., **Pati, S.G.**, Hofstetter, T.B. Characterization of O_2 uncoupling in biodegradation reactions of nitroaromatic contaminants catalyzed by rieske oxygenases. In *Mononuclear Non-heme Iron-dependent Enzymes*. Bridwell-Rabb, J.D., Ed., Methods in Enzymology Vol. 703, Academic Press: Cambridge, MA, United States, **2024**, 3-28.

Pati, S.G., Kohler, H.-P.E., Hofstetter, T.B. Characterization of substrate, co-substrate, and product isotope effects associated with enzymatic oxygenations of organic compounds based on compound-specific isotope analysis. In *Measurement and Analysis of Kinetic Isotope Effects*. Anderson, V.E., Harris, M.E., Eds., Methods in Enzymology Vol. 596, Academic Press: Cambridge, MA, United States, **2017**, 291-329.

Data Sets

de Carvalho, C.F.M., Lehmann, M.F., **Pati, S.G.** Dataset for: Variability in oxygen isotopic fractionation of enzymatic O_2 consumption. *Zenodo*, **2025**, DOI: 10.5281/zenodo.14765061.

Pati, S.G., Brunner, L.M., Ley, M., Hofstetter, T.B. Dataset for: Oxygen isotope fractionation of O_2 consumption through abiotic photochemical singlet oxygen formation pathways. *Zenodo*, **2024**, DOI: 10.5281/zenodo.14267139.

de Carvalho, C.F.M., Lehmann, M.F., **Pati, S.G.** Dataset for: Improving the accuracy of $\delta^{18}O$ and $\delta^{17}O$ values of O_2 measured by continuous-flow isotope-ratio mass spectrometry with a multi-point isotope-ratio calibration. *Zenodo*, **2023**, DOI: 10.5281/zenodo.8043544.

Pati, S.G., Arnold, W.A. Comprehensive screening of quaternary ammonium surfactants and ionic liquids in wastewater effluents and lake sediments. *Data Repository for the University of Minnesota*, **2019**, DOI: 10.13020/ram6-m093.