Monday, 30 May 2022

8:00		**Registration & Coffee**
8:30		**Welcome**
Process tracing in ecology & plant science Christiane Werner (University of Freiburg) Marco Lehmann (WSL)	**8:45**	**A. Kahmen – University of Basel – keynote speaker** Using carbon and oxygen isotopes of herbarium specimen to infer long-term physiological responses of plants to global environmental change
	9:25	**L. Wingate – INRAE – invited speaker** Is a 'black box' approach sufficient to predict the exchange of $CO^{18}O$ and COS between soils and the atmosphere or do we need to dig deeper?
	9:45	**Coffee Break**
	10:45	**C.A. Stricker – US Geological Survey (online)** Fat and fit: diet estimation, macronutrient assimilation, and nutritional implications for an iconic Arctic predator
	11:00	**M. Julien – GFZ Potsdam** Re-evaluation of the ^{13}C isotope fractionation associated with fatty acids biosynthesis by position-specific isotope analysis
	11:15	**L. E. Daber – University of Freiburg** Position-specific isotope labelling gives new insights into chiral monoterpene synthesis
	11:30	**D. B. Nelson – University of Basel** Historic European monthly precipitation isotope time series reconstructions using machine learning
	11:45	**T. Röckmann – Utrecht University** Exploring the potential of $\Delta^{17}O$ in CO_2 for determining mesophyll conductance
12:00		**Lunch**
Food authenticity, forensic & biomedical applications Michèle Lees (Eurofins) Illa Tea (University of Nantes)	**13:30**	**S. Kelly – IAEA – keynote speaker** Improving accessibility to food authentication, using stable isotope analysis, in developing countries: The activities of the joint FAO/IAEA Centre's food safety and control laboratory
	14:10	**M. Straub – University Hospital of Lausanne – invited speaker** Distinct nitrogen isotopic compositions of healthy and cancerous tissue in mice brain and head & neck micro-biopsies
	14:30	**M. Perini – Centro di Trasferimento Tecnologico** Stable isotope ratio analysis to assess pharmaceuticals, cosmetics and dietary supplements authenticity
	14:45	**H. Meijer – University of Groningen** First Use of Triply Labelled Water analysis for energy expenditure measurements in mice
15:00		**Poster Session I (Coffee)**
Computation of isotope effects & enzyme mechanisms Agnieszka Dybala-Defratyka (Lodz University of Technology)	**16:30**	**K. Świderek – Universitat Jaume I – keynote speaker** Towards a new protocol for computer assisted biocatalysts design
	17:10	**P. Paneth – Lodz University of Technology – invited speaker** My 50 years with isotope effects
	17:30	**V. Moliner – Universitat Jaume I** Towards the design of an improved Retro-Aldolase based on QM/MM studies of the reaction catalyzed by different protein scaffolds
	17:45	**I. H. Williams – University of Bath** Computational simulation of kinetic isotope effects for enzymatic N-glycoside hydrolysis
18:00		**Poster Session II (Beverages)**

Session on the occasion of the 70th birthday of Piotr Paneth

Tuesday, 31 May 2022

8:15		**Welcome Coffee**
Advances in analytical instrumentation and methods Matthias Gehre (UFZ) and Béla Tuzson (Empa)	**8:45**	**A. Gilbert – Tokyo Institute of Technology – keynote speaker** Isotopologues of organic molecules: method developments and applications
	9:25	**C. Neubauer – University of Colorado – invited speaker** Discovering isotopic fingerprints anew on bioanalytical mass spectrometers
	9:45	**Coffee Break (Information on the Wednesday Afternoon excursion)**
	10:45	**C. Rennick – National Physical Laboratory (online)** Calibration of Boreas: a new laser-based instrument for *in-situ* automated measurement of $\delta^{13}C$ and $\delta^{2}H$ in methane
	11:00	**T. Csernica – California Institute of Technology** High-Dimensional Isotomics: Observation and Interpretation of Over 100 Isotopic Constraints on Methionine
	11:15	**R. G. H. Marks – University of Essen** How to Couple LC-IRMS with HRMS – A Proof-of-Concept Study
	11:30	**S. Renou – University of Nantes** Towards unbiased ^{13}C isotopic composition in PSIA
	11:45	**B. Tuzson – Empa** Mid-infrared laser spectroscopy coupled to continuous sublimation extraction. A novel method for high-precision greenhouse gas measurements in ice cores
12:00		**Lunch**
Clumped isotopes Stefano Bernasconi (ETH Zürich) Ivan Prokhorov (Empa)	**13:30**	**J. Fiebig – Goethe University of Frankfurt – keynote speaker** Benefits and perspectives of carbonate dual clumped isotope thermometry
	14:10	**M. Clog – University of Glasgow – invited speaker** Robustness of clumped carbonate thermometry in carbonates from the Tara Deep, a large Irish orebody
	14:30	**M. Sivan – Utrecht University** Characterization of microbial methane using clumped isotope measurements
	14:45	**J. Quade – University of Arizona** Carbonate clumped isotope calibration from 6 to 1100°C using an isotope ratio laser spectrometer based on tunable infrared laser spectroscopy
15:00		**Poster Session III (Coffee)**
Origin and evolution of the Earth (planets) & life Huiming Bao (Nanjing University)	**16:30**	**Y. Ueno – Tokyo Institute of Technology – keynote speaker** Tracing oxygen in sulfate using ^{34}S-^{18}O-clumping
	17:10	**J. Hemingway – ETH Zürich – invited speaker** Interpreting triple-oxygen isotope compositions in the geologic sulfur cycle
	17:30	**I. Bobrovskiy – GFZ Potsdam** Compound-specific isotope analysis on phylogenetically specific molecular fossils as a tool to de-convolve the stable carbon isotope record of the deep time
	17:45	**M. H. Thiemens – University of California San Diego** Solar controls of radioactive sulfur isotopes
18:00		**Poster Session IV (Beverages)**

ISI Isotopes
Empa, May 29 – June 3, 2022
Dübendorf / Zürich, Switzerland

Wednesday, 1 June 2022

8:15		**Welcome Coffee**
	8:45	**S. Ono – MIT – keynote speaker** A model for isotopologue signatures of microbial methane to improve source attributions
	9:25	**L. Yu – Tsingua University / Empa – invited speaker (online)** Constraining global N_2O budgets with decadal trends of multiple isotope signatures
	9:45	**A. Matson – Thünen Institute (announcement)** Research Gate Discussion Group: Isotopic tools to study N_2O in soil and aquatic systems
	9:52	**R. Hill-Pearce – National Physical Laboratory (online)** Stable isotope reference materials for climate change monitoring
10:00		**Coffee Break (Information on the Friday Mt. Rigi tour)**
	11:00	**P. M. Homyak – University of California Riverside** Using isotopes to understand N-limitation in dry lands: Unexpected N loss pathways in systems with too little N
	11:15	**A. Hoheisel – University of Heidelberg** Evaluation of six years of continuous $\delta^{13}CH_4$ measurements in Heidelberg, Germany
	11:30	**R. W. van Zwieten – Picarro, Inc. (sponsored)** Committed to Science - Stable isotope analysis with CRDS – practical considerations and use cases
	11:45	**J. Kaiser – University of East Anglia** Polyisotopic carbon dioxide ratios at the coastal Weybourne Atmospheric Observatory (Norfolk, UK)
	12:00	**S. L. Baartman – Utrecht University** Isotopic measurements of carbonyl sulfide (COS): from biosphere to stratosphere
	12:15	**H. Bao – Nanjing University** Atmospheric sulfate of prehuman time in inland northern China
12:30		**Lunch**
15:00		**Afternoon Excursion**
18:00		**Conference Dinner – ETH Zürich**

GLOBAL CHANGE, GREENHOUSE GASES & AEROSOLS
Thomas Röckmann (Utrecht University) and Sakae Toyoda (Tokyo Institute of Technology)

Thursday, 2 June 2022

8:30		**Welcome Coffee**
BIOGEOCHEMISTRY, ELEMENTAL CYCLES AND FATE OF CONTAMINANTS Anat Bernstein (Ben-Gurion University of the Negev) Moritz Lehmann (University of Basel)	**9:00**	**K. L. Casciotti – Stanford University – keynote speaker** Tracing nitrous oxide biogeochemistry in marine oxygen deficient zones using isotopes and isotopomers
	9:40	**C. L. Kelly – Stanford University** Identifying a potentially variable site preference for hybrid nitrous oxide production via isotopomer labeling experiments
	9:55	**Coffee Break**
	11:00	**E. Harris – ETH Zürich** Denitrifying pathways dominate nitrous oxide emissions from managed grassland during drought and rewetting
	11:15	**B. Mayer – University of Calgary** Isotopic tracing of sources and fate of nitrate, sulfate and methane in groundwater in Alberta (Canada)
	11:30	**B. Wolf – Karlsruhe Institute of Technology** Intramolecular N_2O isotopic composition from grassland without preconcentration: interferences correction, nitrification inhibitors, freeze-thaw events and source process identification
	11:45	**A. Danner & G. Rahe – Envicontrol (sponsored)** Analysis of soil respiration with OA-ICOS technology
	12:00	**Lunch**
	13:30	**D. Hunkeler – University of Neuchatel – keynote speaker** Does compound-specific isotope analysis contribute to a new conceptual understanding of the fate of contaminants in the environment?
	14:10	**M. Wiggenhauser – ETH Zürich** Fractionation of stable isotopes of metals and metalloids in plants - copper and cadmium as examples
	14:25	**S.-L. Badea – ICSI** Dehalogenation of α-hexachlorocyclohexane by iron sulfide nanoparticles: Study of reaction mechanism with stable carbon isotopes and pH variations
	14:40	**P. R. Martin – University of Tübingen** Manganese–driven oxidation of aminotris (methylene) phosphonate (ATMP) studied by carbon CSIA
	14:55	**Coffee Break**
	15:55	**S. G. Pati – University of Basel** Oxygen kinetic isotope effects associated with reactions of singlet oxygen in aqueous solutions
	16:10	**C. E. Bopp – EAWAG** Tracing mechanistic adaptations of enzymatic oxygenations of aromatic contaminants using ^{13}C and ^{18}O kinetic isotope effects
	16:25	**J. Hayles – NASA (online)** Constraints on triple oxygen isotope kinetics
	16:40	**M. Elsner – Technical University of Munich** Isotope fractionation reveals limitations and microbial regulation of pollutant biodegradation at low concentrations
16:55		**Goodbye!** **(to all not joining the Friday Mt. Rigi tour)**

Posters

Monday, 15:00–16:30 and 18:00–19:00

Process tracing in ecology & plant science (Poster Session)

Christiane Werner (University of Freiburg) and Marco Lehmann (WSL)

P1	**C. Buchen-Tschiskale – Thünen Institute** Using N_2O isotopocule analysis and ^{15}N tracing approach to gain insights into N_2O source processes in hydroponic tomato cultivation
P2	**R. Well – Thünen Institute** Combining ^{15}N tracing and ^{15}N site preference of N_2O to distinguish production by nitrification and fungal denitrification
P3	**F. Tamburini – ETH Zürich** Oxygen isotopes in phosphate: defining potentials and limitations for environmental studies
P4	**R. A. Werner – ETH Zürich** Intramolecular ^{13}C patterns of plant glucose convey environmental and metabolic information
P5	**F. Damak – Tokyo Institute of Technology** Insights into nitrous oxide reduction by soybean inoculated with Bradyrhizobium from concentration and isotopocule analyses in a field
P6	**S. N. Ladd – University of Freiburg** Leaf-level metabolic changes in daytime respiration and isoprenoid synthesis during drought determined by position-specific ^{13}C-pyruvate labeling
P7	**C. Werner – University of Freiburg** Whole ecosystem $^{13}CO_2$ and $^{2}H_2O$ Pulse-Labelling to investigate carbon allocation, CO_2 and VOC emissions and the role of deep water reserves during drought
P8	**J. Baan – University of Basel** Comparing hydrogen isotope compositions of different lipid compounds across species to address possible origin of variation

Food authenticity, forensic & biomedical applications (Poster Session)

Michèle Lees (Eurofins) and Illa Tea (University of Nantes)

P9	**C. Citérin – Nantes Université** Isotopic signature of ^{13}C and ^{15}N natural abundance in breast cancer patients
P10	**M. Couton – Nantes Université** ^{15}N-position-specific isotope analysis by isotope ratio mass spectrometry (PSIA-IRMS)
P11	**M. Perini – Centro di Transferimento Technologico** Isotope ratio mass spectrometry to detect differences in four compartments of Simmental cows fed on C3 and C4 diets
P11/2	**P. Paneth – Lodz University of Technology** The first oxygen stable isotopes assessment in 'in vivo' cancer tissues – a pilot study.

Computation of isotope effects & enzyme mechanisms (Poster Session)

Agnieszka Dybala-Defratyka (Lodz University of Technology)

P12	**L. Chai – TU Munich** Metabolic mechanism of sulfonamide cleavage: a combined computational and experimental study on sulfamethoxazole
P13	**A. Dybala-Defratyka – Lodz University of Technology** Isotope effects on vaporization of organic compounds from aqueous solution – insight from experiment and computations
P14	**L. Pennacchio – University of Copenhagen** First principles model of isotopic fractionation in formaldehyde photolysis: Wavelength and pressure dependence

Posters

Monday, 15:00–16:30 and 18:00–19:00

Advances in analytical instrumentation and methods (Poster Session)

Matthias Gehre (UFZ) and Béla Tuzson (Empa)

P15 **F. Antritter – TU Munich**
Reducing the unwanted: selectivity of various solid phase extraction sorbents in relation to dissolved organic matter

P16 **A. Canavan – TU Munich**
Position-specific isotope analysis using ^{13}C-labels on sulfamethoxazole

P17 **A. Tafa – TU Munich**
Suitability of passive sampling for compound-specific isotope analysis of micropollutants in aquatic environments

P18 **R. Bakkour – TU Munich**
Universal vs. selective sorbents for targeted isotope analysis of aquatic contaminants

P19 **C. Wabnitz – TU Munich**
Coupling a quartz crystal microbalance with liquid chromatography for online NOM monitoring

P20 **S. Leitner – Institute of Soil Research**
A UAV-based sampling system to analyze greenhouse gases and volatile organic carbons encompassing compound specific stable isotope analysis

P21 **E. P. Mueller– California Institute of Technology**
High-precision ESI-Orbitrap MS measurements of hydrogen isotope compositions from organic molecules

P22 **A. Hilkert – Institute of Soil Research**
Comprehensive isotope ratio MS with electrospray-Orbitrap

P23 **M. Öztopark – Royal Netherlands Institute for Sea Research**
Investigating the intramolecular isotopic structure of isoprenoids via ultra high resolution APCI - Orbitrap mass spectrometry

P24 **G. S. Remaud – Nantes University**
Exploring the potential of ^{17}O NMR for intramolecular ^{17}O isotope profile: application to vanillin origin discrimination

P25 **S. Renou – Nantes University**
How to determine the intramolecular ^{13}C composition on low amount of glucose using irm ^{13}C-NMR

P26 **R. P. J. Moonen – Utrecht University**
First results of CO_2 and H_2O Isotope-Flux Measurements a semi-arid area with large scale irrigation

P27 **G. A. Adnew – Utrecht University**
Temperature dependence of isotopic fractionation in the CO_2-O_2 isotope exchange reaction

P28 **E. Safi – National Physical Laboratory**
Fractionation effects during methane separation from ambient air for high-precision optical analysis of $\delta^{13}C$ and $\delta^{2}H$

P29 **A. Th. Aerts-Bijma – University of Gröningen**
Where do IRMS's go wrong? $\delta^{18}O$ SLAP determined at -56.3‰

P30 **K. Huang – Empa**
A novel automated technique for simultaneous online analysis of ^{15}N in ammonium, nitrite, and nitrate

P31 **K. Zeyer – Empa**
Real-time analysis of $\delta^{13}C$- and δD-CH_4 in ambient air with a QCL based absorption spectrometer: Method development

P32 **M. Lehmann – WSL**
The hydrogen isotopic composition of plant carbohydrates – Advancement in methods and interpretation

P33 **S. Hugger – University of Basel**
Method optimization for plant sugar purification and compound-specific hydrogen isotope analysis

P33/2 **S. G. Pati – University of Basel**
δ-scale calibration for stable isotope analysis of O_2 by continuous flow IRMS from -10 to +95 ‰ with in-vitro photosynthesis experiments **P58**

Posters

Tuesday, 15:00–16:30 and 18:00–19:00

Clumped isotopes (Poster Session)

Stefano Bernasconi (ETH Zürich) and Ivan Prokhorov (Empa)

P34 **A. Nataraj – Empa**
Quantum cascade laser absorption spectrometer with a low temperature multipass cell for precision clumped $^{12}C^{18}O_2$ and position specific isotope analysis

P35 **I. Prokhorov – Empa**
Concordant optical clumped isotope thermometry of methane

P36 **H. Eckhardt – University of Heidelberg**
Atmospheric CO_2 sources with specific Δ_{47} signals under mixing conditions

P37 **N. Looser – ETH Zürich**
Clumped isotope reordering in belemnite and optical calcites: Towards material-specific reordering kinetics

P38 **N. Zhang – Tokyo Institute of Technology**
Abiotic methane formation in nature: information from clumped isotope analysis of laboratory synthesized methane

Origin and evolution of the Earth (planets) & life (Poster Session)

Huiming Bao (Nanjing University)

P39 **L. Liu – Australian National University**
SHRIMP-SI quadruple sulfur isotopic compositions of two generations of pyrite in the 3.49 Ga dresser formation

Global change, greenhouse gases & aerosols (Poster Session)

Thomas Röckmann (Utrecht University) and Sakae Toyoda (Tokyo Institute of Technology)

P40 **H. A. Scheeren – University of Gröningen**
Measuring the stable isotopic composition of pure CO_2 samples on a dual-laser absorption spectrometer using a back-dilution method to obtain dry ambient conditions

P41 **P. M. Steur – University of Gröningen**
A four-year record (2017-2021) of $\Delta^{17}O$ in atmospheric CO_2 from Lutjewad station (NL)

P42 **M. Fatima – VTT**
Comparison of laser sources and driver electronics for optical isotope ratio spectroscopy

P43 **S. Toyoda – Tokyo Institute of Technology**
Spacio-temporal distributions of atmospheric nitrous oxide and its isotopocules

P44 **A. Matson – Thünen Institute**
Research Gate Discussion Group: Isotopic tools to study N_2O in soil and aquatic systems

Posters

Tuesday, 15:00–16:30 and 18:00–19:00

Biogeochemistry, elemental cycles and fate of contaminants (Poster Session)

Anat Bernstein (Ben-Gurion University of the Negev) and Moritz Lehmann (University of Basel)

P45 **K. Müller – TU Munich**
Applicability of a reverse stable isotope labeling approach to show biodegradation of microplastics on a single-cell level

P46 **A. Matson – Thünen Institute**
Using depth profiles and natural abundance stable isotopes to determine N_2O processes in agricultural soils

P47 **K. Kourtaki – University of Tübingen**
Application of compound-specific carbon isotope analysis on aerobic biotransformation of glyphosate

P48 **A. Röhnelt – University of Tübingen**
Heterogenous oxidation of aminopolyphosphonates and AMPA at manganese oxide surfaces studied by carbon LC-IRMS

P49 **O. Boukaroum – Aix-Marseille University**
Significant ^{2}H and ^{13}C isotope fractionation during volatilisation and diffusion of hydrocarbons in soil

P50 **P. Höhener – Aix-Marseille University**
DECiSIvE - Tracking degradation of soil pollutants with multi-elemental compound-specific isotope analysis

P51 **M. Alvarez-Salas – ETH Zürich**
Stable isotopes of oxygen: the key to understand the soil fate of fertilizer-derived phosphorus?

P52 **E. Stoll – University of Innsbruck**
New insights into climate change-driven soil N_2O production and emissions in managed montane grassland

P53 **M. Vinyes-Nadal – University of Barcelona**
Assessing methoxychlor contamination and natural attenuation in a polluted aquifer using carbon compound specific isotope analyses

P54 **D. Lewicka-Szczebak – University of Wrocław**
Combining isotope mixing and fractionation with a new modelling tool applying the Monte Carlo approach

P55 **M. Bucha – University of Wrocław**
Tracing anaerobic decomposition of lactate, butyrate, propionate, and acetate by means of carbon isotopic analyses of products CH_4, CO_2, and DIC in the continuous-flow open systems

P56 **P. M. Magyar – University of Basel**
Constraining interplay between kinetic and equilibrium isotope effects during anammox in a wastewater treatment system

P57 **T. Einzmann – University of Basel**
Understanding biogeochemical controls on nitrous oxide production and consumption in Lake Lugano, Switzerland

P58 **S. G. Pati – University of Basel**
δ-scale calibration for stable isotope analysis of O_2 by continuous flow IRMS from -10 to +95 ‰ with in-vitro photosynthesis experiments **P33/2**

P59 **C. F. M. de Carvalho – University of Basel**
Oxygen isotope fractionation during enzymatic O_2 consumption reactions

P60 **T. Kuder – University of Oklahoma**
Hydrogen isotope exchange between trichloroethene and water under mild environmental conditions – implications for the use of hydrogen CSIA in contaminated site assessment

P61 **N. Gluschankoff – Stanford University**
Isotopic analysis of nitrous oxide during El Niño and La Niña in the Eastern tropical South Pacific

P62 **J. Mohn – Empa**
Tracing N_2O formation in full-scale wastewater treatment with natural abundance isotopes