

## Isotopes 2015 – Isotope effects across disciplines

<b>Sunday, June 21</b>	
16:00-18:00	Arrivals and registration
18:30-20:00	Welcome mixer
20:00-20:15	Opening words
20:15-21:00	<b>Opening lecture: Yehoshua Kolodny</b> – Hebrew University
<b>Monday, June 22</b>	
<b>09:00-11:00</b>	<b>Morning session: Medical use of stable isotopes (Chair: Anil Modak – Cambridge Isotopes)</b>
09:00-09:30	Keynote lecture: <b>Yaron Ilan</b> – Hadassah Medical Center <i>Measurement of the <math>^{13}\text{CO}_2/^{12}\text{CO}_2</math> ratio in exhaled air following oral administration of <math>^{13}\text{C}</math>-Methacetin using the non-invasive BreathID®: A novel method for assessment of liver function of patients with acute and chronic liver disorders</i>
09:30-10:00	Keynote lecture: <b>Anil S. Modak</b> – Cambridge Isotopes <i>Companion Diagnostics (CDx) for personalizing medication</i>
10:00-10:20	Contributed lecture: <b>Martin Klieber</b> – Cambridge Isotopes <i>Cytochrome P450 2C19 phenoconversion by routinely prescribed proton pump inhibitors omeprazole and esomeprazole: clinical implications for personalized medicine</i>
10:20-10:40	Contributed lecture: <b>Yliya Rabotjagova</b> – Crimean State Medical University <i>Evaluation of changes to CYP2C19 enzyme activity (phenotype) with the Pantoprazole-<math>^{13}\text{C}</math> breath test after initiating PPI therapy in GERD patients</i>
10:40-11:00	Contributed lecture: <b>Illa Tea</b> – University of Nantes (CEISAM-CNRS)/Australian National University <i>Isotopomics in breast cancer</i>
<b>11:00-11:30</b>	<b>Coffee break</b>
<b>11:30-13:30</b>	<b>Late morning session: Isotopes in environmental sciences (Chair: Tomasz Kuder – University of Oklahoma)</b>
11:30-12:00	Keynote lecture: <b>Martin Elsner</b> – Helmholtz Zentrum München <i>Current Challenges in Isotope Studies of Environmental Contaminants: Multielement Isotope Analysis and Investigations of Micropollutants</i>
12:00-12:20	Contributed lecture: <b>Maxime Julien</b> – University of Nantes <i>Modelling of position-specific isotope effects measured by isotopic quantitative <math>^{13}\text{C}</math> NMR occurring during volatilization of environmental pollutants</i>
12:20-12:40	Contributed lecture: <b>Martin Mihaljevic</b> – Charles University in Prague <i>Tracing Cu and Pb dynamics in semi-arid soils near mine</i>

	<i>tailings (Kombat, Namibia) using stable isotopes</i>
12:40-13:00	Contributed lecture: <b>Xi Wei</b> – Helmholtz Center for Environmental Research <i>Characterization of phenols biodegradation by compound specific stable isotope analysis</i>
13:00-13:15	Contributed lecture: <b>Noa Balaban</b> – Ben-Gurion University <i>Isotopic fractionation during biodegradation of brominated aliphatic flame retardants</i>
13:15-13:30	Contributed lecture: <b>Miao Yu</b> – State Key Laboratory of Environmental Chemistry and Ecotoxicology <i>Organic Stable Isotope Analysis with GC-qMS for PBDEs in a molecular view</i>
<b>13:30-15:00</b>	<b>Lunch</b>
<b>15:30-17:30</b>	<b>Afternoon session: Isotopes in biological sciences I (Chair: Miryam Bar-Matthews – Geological Survey of Israel)</b>
15:30-16:00	Keynote lecture: <b>Ariel Anbar</b> – Arizona State University <i>Developing a clinically useful calcium isotope biomarker</i>
16:00-16:30	Keynote lecture: <b>Justine P. Roth</b> – Johns Hopkins University <i>Mechanistic Studies of Dioxygenase Activity in Cyclooxygenase-2</i>
16:30-16:50	Contributed lecture: <b>Anton Eisenhauer</b> – Helmholtz Centre of Ocean Research Kiel <i>Testing Ca Isotope Fractionation in mini-pigs as an animal model for trace element cycling in humans</i>
16:50-17:10	Contributed lecture: <b>Johanna Irrgeher</b> – University of Nat. Res. Appl. Life Sci. Vienne <i>Sr isotopes as tracers in archeological sciences</i>
17:10-17:30	Contributed lecture: <b>Caroline Ek</b> – Stockholm University <i>Stable isotope incorporation in Daphnia in response to toxic exposure – potential implications for estimating Trophic Magnification Factors</i>
<b>18:30-19:30</b>	<b>Dinner</b>
<b>20:00-22:00</b>	<b>Mix time</b>
<b>Tuesday, June 23</b>	
<b>09:00-11:00</b>	<b>Morning session: Isotopes in biological sciences II (Chair: Agnieszka Dybala-Defratyka, Lodz University of Technology)</b>
09:00-09:30	Keynote lecture: <b>Amnon Kohen</b> – University of Iowa <i>Interpretation of Temperature Dependence of Kinetic Isotope effects</i>
09:30-10:00	Keynote lecture: <b>Jeroen Dickschat</b> – University of Bonn <i>Terpenes from Microorganisms</i>
10:00-10:20	Contributed lecture: <b>Katarzyna Romek</b> – Lodz University of Technology <i>Position-specific isotope analysis - a retro-biosynthetic approach to predicting biosynthetic pathways?</i>

10:20-10:40	Contributed lecture: <b>Dominika Lewicka-Szczebak</b> – Thünen <i>The Mechanism of Oxygen Isotopic Fractionation During N<sub>2</sub>O Production by Denitrification</i>
10:40-11:00	Contributed talk: <b>Lynn Kamerlin</b> – Uppsala University <i>Phosphoryl and Sulfuryl Transfer Reactions: Challenges in Interpreting Experimental and Theoretical Data</i>
<b>11:00-11:30</b>	<b>Coffee break</b>
<b>11:30-13:30</b>	<b>Late morning session: Theoretical approaches for calculations of isotope effects I (Chair: Lynn Kamerlin – Uppsala University)</b>
11:30-12:00	Keynote lecture: <b>Iñaki Tuñón</b> – Universitat de Valencia <i>Adiabatic and Nonadiabatic Hydride Transfer in Formate Dehydrogenase</i>
12:00-12:30	Keynote lecture: <b>Johannes Kaestner</b> – University of Stuttgart <i>Atom Tunneling: from Astrochemistry to Enzymes</i>
12:30-12:50	Contributed lecture: <b>Ian Williams</b> – University of Bath <i>Isotope Effect Calculations for Methyl Transfer</i>
12:50-13:10	Contributed lecture: <b>Sebastian Kozuch</b> – Ben-Gurion University <i>Heavy Atom Tunneling: Stability, Selectivity, and some Isotopes</i>
13:10-13:30	Contributed lecture: <b>Agnieszka Dybala-Defratyka</b> - Lodz University of Technology <i>Kinetic Isotope Effects Accompanying Degradation of Hexachlorocyclohexanes by the LinA and LinB Dehalogenases. A Computational Study</i>
<b>13:30-15:00</b>	<b>Lunch</b>
<b>15:00-19:00</b>	<b>Excursion - Jerusalem Old City</b>
<b>19:00-20:30</b>	<b>Dinner</b>
<b>Wednesday, June 24</b>	
<b>09:00-11:00</b>	<b>Morning session: Isotope effects in chemical processes: organic and inorganic reactions (Chair: Zeev Aizenshtat – Hebrew University)</b>
09:00-09:30	Keynote lecture: <b>Peter Schreiner</b> – University of Giessen <i>Tunneling Control of Chemical Reactions</i>
09:30-10:00	Keynote lecture: <b>Piotr Paneth</b> – Lodz University of Technology <i>Isotopic fractionation - from basic science to applications</i>
10:00-10:20	Contributed lecture: <b>Thomas Hofstetter</b> – EAWAG <i>Isotope Fractionation Associated with the Direct Photolysis of Chloroanilines</i>
10:20-10:40	Contributed lecture: <b>Mahmoud Alkhatib</b> – Helmholtz Centre for Ocean Research <i>Calcium and Strontium Isotope measurement on artificially precipitated calcium carbonate</i>
10:40-11:00	Contributed lecture: <b>Yevgeni Zakon</b> – Geological Survey of

	Israel <i>Dual carbon-bromine isotope effect during photolysis of brominated phenols</i>
<b>11:00-11:30</b>	<b>Coffee break</b>
<b>11:30-13:30</b>	<b>Late morning session: Isotopes in Earth and planetary sciences (Chair: Alon Amrani – Hebrew University)</b>
11:30-12:00	Keynote lecture: <b>James Farquhar</b> – University of Maryland <i>How did the isotopic composition of oceanic sulfate evolve in the late Archean?</i>
12:00-12:30	Keynote lecture: <b>Hagit Affek</b> – Yale University <i>Carbonate clumped isotope geothermometry: principles, applications, and challenges</i>
12:30-12:50	Contributed lecture: <b>Miryam Bar-Matthews</b> – Geological Survey of Israel <i>Stable Isotope frontiers in paleo-hydrological studies using speleothems</i>
12:50-13:10	Contributed lecture: <b>Lubna Shawar</b> – Hebrew University <i>Compound specific sulfur isotope approach to study the redox cycling during the deposition of Senonian oil shale in the Late Cretaceous Tethyan margin, Israel</i>
13:10-13:30	Contributed lecture: <b>Monika Cieżka</b> – University of Wrocław <i>Assessing anthropressure in the Świętokrzyski National Park: An approach coupling stable isotope and Electron Paramagnetic Resonance (EPR) analyses of lichen (<i>Hypogymnia physodes</i>)</i>
<b>13:30-15:00</b>	<b>Lunch</b>
<b>15:30-16:00</b>	Special Lecture in memory of Prof. J. Gatt – <b>Dan Yakir</b> , Weizmann Institute of Science <i>Association between <math>18\Delta</math> and Carbonyl Sulfide Uptake and during <math>CO_2</math> exchange between the atmosphere and land plants</i>
<b>16:00-18:00</b>	<b>Poster session</b>
<b>18:30-22:00</b>	<b>Gala Dinner (The Israel Museum)</b>
<b>Thursday, June 25</b>	
<b>08:45-11:00</b>	<b>Morning session: Stable isotopes (traditional and non-traditional) analyses (Chair: Alexey Kamysny – Ben-Gurion University)</b>
08:45-09:15	Keynote lecture: <b>Thomas Prohaska</b> – University of Nat. Res. Appl. Life Sci. Vienne <i>Spiking, marking and tracing – Isotopic tools as specific monitors and markers of elemental fluxes</i>
09:15-9:45	Keynote lecture: <b>Hans Eggenkamp</b> – Onderzoek & Beleving <i>Comparing stable chlorine and bromine isotope analysis; Techniques and directions for future research</i>
9:45-10:05	Contributed lecture: <b>Tomasz Kuder</b> – University of

	Oklahoma <i>Studies of VOCs Contaminants: Overcoming Analytical Limitations of CSIA</i>
10:05-10:25	Contributed lecture: <b>Pierrick Nun</b> – University of Nantes <i>Applications of <math>^{13}\text{C}</math> isotopic quantitative NMR for position-specific measurements (PSIA): from biosynthetic pathway to environmental studies</i>
10:25-10:45	Contributed lecture: <b>Alex Wolf</b> – Israel Atomic Energy Commission <i>Analyses of stable isotopes-a multiple application opportunity</i>
10:45-11:00	Contributed lecture: <b>Rob Peters</b> – Picarro, Inc. <i>Cavity Ring-Down Spectroscopy as a tool for partitioning evaporation and transpiration using water isotopes</i>
<b>11:00-11:30</b>	<b>Coffee break</b>
<b>11:30-13:30</b>	<b>Late morning session: Theoretical approaches for calculations of isotope effects II (Chair: Vicente Moliner – Universitat Jaume I)</b>
11:30-12:00	Keynote Lecture: <b>Steve Schwartz</b> – University of Arizona <i>Protein Dynamics, Heavy Enzymes, and Protein Design for Enzymatic Catalysis</i>
12:00-12:30	Keynote lecture: <b>Mike Webb</b> – Caltech <i>Path-integral methods for evaluating equilibrium isotope effects: applications to clumped and position-specific stable isotope studies</i>
12:30-12:50	Contributed lecture: <b>Yuval Shagam</b> – Weizmann Institute of Science <i>Observation of the isotope effect in sub-kelvin reactions</i>
12:50-13:10	Contributed lecture: <b>Debasish Mandal</b> – Hebrew University <i>Kinetic Isotope Effect is a Sensitive Probe of Spin State Reactivity in C-H activation of non-heme Fe(IV)O oxidants with Hydrocarbon</i>
13:10-13:30	Contributed lecture: <b>Josef Yellin</b> – Hebrew University <i>Isotope effects in atomic structure</i>
<b>13:30-15:00</b>	<b>Lunch</b>
<b>15:30-17:50</b>	<b>Afternoon session: Isotopes in marine sciences and hydrology (Chair: Anton Eisenhauer – Helmholtz Centre for Ocean Research Kiel)</b>
15:30-16:00	Keynote lecture: <b>Mark Altabet</b> – University of Massachusetts <i>Deciphering the Ocean's Nitrogen Cycle using Stable Isotope Ratios</i>
16:00-16:30	Keynote lecture: <b>Orit Sivan</b> – Ben-Gurion University <i>The use of multi-isotope measurements to study anaerobic methane oxidation (AOM) process in marine and freshwater sediments</i>
16:30-16:50	Contributed lecture: <b>Alan Matthews</b> – Hebrew University <b>Contrasting anoxic conditions in Eastern</b>

	<i>Mediterranean Sapropels S1 and S5 revealed by Fe and Mo isotopes and chemical element proxies</i>
16:50-17:10	Contributed lecture: <b>Jegathambal P</b> – Karunya University <i>Environmental Isotopes and Hydrogeochemical Parameters as Indicators of Groundwater Recharge in Semiarid Regions</i>
17:10-17:30	Contributed lecture: <b>Noa Fruchter</b> – Hebrew University <i>Lake Kinneret as a natural laboratory to study the carbonate system using <math>^{88}\text{Sr}/^{86}\text{Sr}</math> fractionation in authigenic inorganic calcite</i>
17:30-17:50	Contributed lecture: <b>Alexey Kamyshny</b> – Ben-Gurion University <i>Sulfur cycling in a freshwater lake with sub-millimolar sulfate concentrations: constraints from sulfur isotope composition of hydrogen sulfide, elemental sulfur, and sulfate</i>
17:50-18:00	<b>Closing remarks</b>
<b>18:30-19:30</b>	<b>Dinner</b>
<b>20:00-22:00</b>	<b>Mix time</b>
<b>Friday, June 26</b>	
<b>09:00-11:00</b>	<b>Excursion – The Museum of Islamic Art</b>