

# Cajetan Neubauer

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## Main Expertise

Isotopic structure of biomolecules and oxyanions, rates of metabolite production in cells and microbiomes, stable isotopes, diagnostic biomarkers, enzyme mechanisms, structural biology, mass spectrometry

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## Research Positions

### University of Colorado Boulder / Research Faculty

Since Jul 2020 | Department of Earth Science | Boulder, CO

Research: Stable isotope analyzer for water-soluble compounds

### Thermo Fisher Scientific / Guest Scientist & Consultant

Feb 2020 - 2024 | Bremen, Germany

Research: R&D for new stable isotope mass spectrometry methods

### California Institute of Technology / Visiting Scientist

Since Jun 2019 | Div. of Geological and Planetary Sciences | Pasadena, CA

### Hanse-Wissenschaftskolleg (HWK) / Senior Fellow

Jun 2019 - Jun 2020 | HWK Institute for Advanced Study | Germany

Research: Biosynthesis of an unusual microbial lipid found in marine sediments

Hosting Lab: Organic geochemistry group (MARUM, Bremen)

### California Institute of Technology / Postdoctoral Researcher

Jan 2012 - May 2019

Research: Microbiology, lipids, mass spectrometry, stable isotopes

Hosting Labs: Prof Dianne Newman (2012-18), Prof John Eiler (2018/19)

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## Education

### MRC Laboratory of Molecular Biology / [PhD thesis](#)

May 2007 - Dec 2011 | Medical Research Council & Cambridge University, UK

Research: Structure of ribosomal RNA/protein complexes.

Adviser: Dr Venki Ramakrishnan

### Max Planck Institut für Biochemie / [Research Assistant](#)

Oct 2006 - Apr 2007 | Munich, Germany

Research: Cryogenic electron microscopy, type III secretion in *Salmonella*

Adviser: Prof Wolfgang Baumeister

### Max Planck Institut für Biochemie / [MSc thesis](#)

Jan - Sep 2006 | Munich, Germany

Research: Protein crystallography, Alzheimer's disease

Advisers: Prof Wolfram Bode, Prof Robert Huber

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## Current Research

**Isotopic structure of nitrate:** We have recently developed a new approach to quantify the stable isotopic content of oxyanions. The technique is based on electrospray Orbitrap mass spectrometry and measures intact molecules. Using nitrate as a model compound, I am assembling a cross-functional team to bridge this potentially transformative technology to environmental science applications.

**Industrially-synthesized methionine in humans:** More than 1 million tons of methionine are fed annually as growth promoter to livestock. Newly emerging biomedical data indicate that excess input of this essential amino acid into the world food supply warrants attention. We use a novel isotope mass spectrometry method to quantify the fraction of methionine in humans that originates from petrochemical synthesis.

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## Public speaking

Conferences, Trainings and Lectures (selection)

**American Society for Mass Spectrometry (ASMS Annual Conference)**  
2024 & 2025, Fundamentals Interest Group Workshop

**ISI + Isotopes (11th International Symposium on Isotopomers)**  
2024, Lecture, Tokyo, Japan

**JESIUM (Joint European Stable Isotope Users Meeting)**  
2022, Lecture, Kuopio, Finland

**Workshop on Stable Isotope Analytics**  
2021, Organizer | HWK Institute for Advanced Study

**Department seminars**  
2021, Lecture | ISAS Institute for Analytical Sciences

**Chinese Bioorganic Geochemistry Symposium (BOGC8)**  
2021, Lecture (online)

**NASA Workshop on Isotopologue Research**  
2019, Lecture | Pennsylvania State University

**Department seminars**  
2019, Lectures | University of Delaware & Stanford University

**Geobiology seminar**  
2019, Lecture | University of Colorado Boulder

**Los Angeles Metropolitan Mass Spectrometry Meeting**  
2019, Lecture | UC Riverside

**Southern California Geobiology Symposium**  
2019, Lecture

**MSACL Annual Congress in Clinical Mass Spectrometry**  
2019, Lecture | 'Scanning the Stable Isotopic Structure of Molecules by Tandem

Mass Spectrometry'

2019, Training | 'A Comprehensive Review of Clinical Mass Spectrometry Technology & Techniques'

### **Benchmarking of ESI-Orbitrap MS for isotope analysis**

2017, R&D | Thermo Scientific, San Jose

### **Department seminars**

2016, Lectures | Trinity College Dublin | National University of Singapore | National University of Malaysia

### **LipidMaps Annual Meetings**

2014 - 2016, Conferences

### **International Singapore Lipid Symposium**

2015, Lecture

### **Secondary Metabolites Workshop**

2015, Training | DOE Joint Genome Institute

### **Fellowship conferences**

2014, Lectures | EMBO US Meeting | Boehringer Foundation US Meeting

### **EMBO Laboratory Management Course**

2014, Training | Heidelberg, Germany

### **GRC Organic Geochemistry**

2014, Conference

### **Microbial Diversity Course**

Jun & Jul 2013, Training | Marine Biological Laboratory

### **Summer School of Molecular and Theoretical Biology**

Aug 2013, Teaching | Pushchino, Russia

### **Meeting of the American Society of Microbiology**

2011 & 2012, Conferences

### **Invited seminars**

2011, Lectures | Max Delbrück Center Berlin | Princeton University | University of Washington | California Institute of Technology

### **European Bioinformatics Institute Summer School**

2010, Training

### **Invited seminars**

2010, Lectures | European Molecular Biology Laboratory (EMBL) | Uppsala University | Tsinghua University

### **Seminar at the Indian Institute of Science**

2008, Lecture

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## **Teaching**

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### **Isotopes 101 workshop / [Mass Spectrometry & Advances in the Clinical Lab \(MSACL\)](#)**

Sep 2025, Montreal, Canada

### **Project Lead & Lecturer / [Summer School for Molecular and Theoretical Biology](#)**

Jul & Aug 2013 | Pushchino, Russia

Responsibilities: Leader of a research lab in environmental microbiology.  
Geobiology lecture series. [More info](#)

## Teaching Assistant / Introductory Biology

2012 | California Institute of Technology

Responsibilities: Teaching weekly recitation sessions.

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## Publications

Reed NW, Christensen CM, Surratt JD, McGlynn SE, Wing BA, [Neubauer C](#), Tolbert MA, Browne EC (2025) An Archean atmosphere rich in sulfur biomolecules. *Proc. Natl. Acad. Sci. U.S.A.* [\[Link\]](#)

Bernet NM, Soldini C, Felder TMO, Lapčíková K, [Neubauer C](#), Queen WL, Kaegi R, Tamburini F, Hofstetter TB (2025) Oxygen isotope analyses of phosphate and organophosphorus compounds by electrospray ionization Orbitrap mass spectrometry. *Analytical Chemistry* [\[Link\]](#)

Hong Y, Zhu L, Crocker DR, Liu T, Wang Z, Wei Z, Yu C, Wei Y, Yan H, Johnston DT, Kohl IE, Peng Y, Hilkert A, [Neubauer C](#), Hattori S (2025) Triple oxygen isotope analysis of methanesulfonate using the SO<sub>3</sub><sup>-</sup> fragment in ESI-Orbitrap-MS. *Analytical Chemistry* [\[Link\]](#)

Kantnerová K, Kuhlbusch N, Juchelka D, Hilkert A, Kopf SH, [Neubauer C](#) (2024) A guide to precise measurements of isotope abundance by ESI-Orbitrap MS. *Nature Protocols* [\[Link\]](#)

[Neubauer C](#), Kantnerová K, Julien M, Öztoprak M, Lamothe A, Hilkert A, Juchelka D, Hinrichs K-U, Elvert M, Bakkour R, Hattori S, Dittmar T, Heuer V, Schouten S, Elsner M (Invited perspectives article; in review). Discovering nature's fingerprints: isotope ratio analysis on bioanalytical mass spectrometers. *Journal of American Society for Mass Spectrometry*

Boettger JD, [Neubauer C](#), Kopf SH, Kubicki JD (2022) Microbial Denitrification: Active Site and Reaction Path Models Predict New Isotopic Fingerprints. *ACS Earth and Space Chemistry* [\[Link\]](#)

Coffinet S, Mühlhena L, Lipp JS, Weil M, Neubauer C, Urich T, Hinrichs K-U (2022) Evidence for enzymatic backbone methylation of the main membrane lipids in the archaeon *Methanomassiliicoccus luminyensis*. *Applied and Environmental Microbiology* [\[Link\]](#)

[Neubauer C](#), Landecker H (2021) A planetary health perspective on synthetic methionine: Implications of opening the tap on a historically limiting nutrient. *Lancet Planetary Health* [\[Link\]](#)

Hilkert A, Böhlke JK, Mroczkowski SJ, Fort KL, Aizikov K, Wang XT, Kopf SH, [Neubauer C](#) (2021) Exploring the potential of Electrospray-Orbitrap for stable isotope analysis using nitrate as a model. *Analytical Chemistry* [\[Link\]](#)

[Neubauer C](#), Cremiere A, Wang XT, Thiagarajan N, Sessions AL, Adkins JF, Dalleska NF, Turchyn AV, Clegg JA, Moradian A, Sweredoski MJ, Garbis SD, Eiler JM (2020) Stable isotope analysis of intact oxyanions using electrospray Orbitrap mass spectrometry. *Analytical Chemistry* [\[Link\]](#)

[Neubauer C](#), Sweredoski MJ, Moradian A, Newman DK, Robins RJ, Eiler JM (2018). Scanning the isotopic structure of molecules by tandem mass spectrometry. *Int J Mass Spec.* [\[Link\]](#) (Patent pending)

Neubauer C, Kasi AS, Grahl N, Sessions AL, Kopf SH, Kato R, Hogan DA, Newman DK (2018). Refining the application of microbial lipids as tracers of *Staphylococcus aureus* growth rates in cystic fibrosis sputum. *J Bacteriology*. [\[Link\]](#) [\[Commentary\]](#)

Neubauer C, Sessions AL, Booth IR, Bowen BP, Kopf SH, Newman DK, Dalleska NF (2018). Towards measuring growth rates of pathogens during infections by D<sub>2</sub>O-labeling lipidomics. *Rapid Commun Mass Spectrom*. [\[Link\]](#)

Newman DK, Neubauer C, Ricci JN, Wu C-H, Pearson A (2016). Cellular and molecular biological approaches to interpreting ancient biomarkers. *Annu Rev Earth Planet Sci*. [\[Link\]](#)

Neubauer C, Dalleska NF, Cowley ES, Shikuma NJ, Wu C-H, Sessions AL, Newman DK (2015). Lipid remodeling in *Rhodopseudomonas palustris* TIE-1 upon loss of hopanoids and hopanoid methylation. *Geobiology*. [\[Link\]](#)

Voorhees RM, Mandal D, Neubauer C, Köhrer C, RajBhandary UL, Ramakrishnan V (2013). The structural basis for specific decoding of AUA by isoleucine tRNA on the ribosome. *Nat Struct Mol Biol*. [\[Link\]](#)

Neubauer C, Gillet R, Kelley AC, Ramakrishnan V (2012). Decoding in the absence of a codon by tmRNA and SmpB in the ribosome. *Science*. [\[Link\]](#)

Neubauer C, Gao Y-G, Andersen KR, Dunham CM, Kelley AC, Hentschel J, Gerdes K, Ramakrishnan V, Brodersen DE (2009). The structural basis for mRNA recognition and cleavage by the ribosome-dependent endonuclease RelE. *Cell*. [\[Link\]](#)

Weixlbaumer A, Jin H, Neubauer C, Voorhees RM, Petry S, Kelley AC, Ramakrishnan V (2008). Insights into translational termination from the structure of RF2 bound to the ribosome. *Science*. [\[Link\]](#)

Klages J, Neubauer C, Coles M, Kessler H, Luy B (2005). Structure Refinement of Cyclosporin A in chloroform by using RDCs measured in a stretched PDMS-gel. *Chembiochem*. [\[Link\]](#)

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