



Annual (Q)SAR User Meeting

*Exploring Applications
in Computational Toxicology*

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17 April 2026

Introduction

Welcome to the MultiCASE Annual (Q)SAR User Meeting, a great opportunity to come together and explore the latest innovations in computational toxicology. Today's discussions will include ICH M7, software updates across our Desktop and Cloud platforms, nitrosamine evaluations, immunogenicity, bioavailability, and general toxicity, including extractables and leachables (E&L).

Who you'll meet from MultiCASE



Dr. Suman Chakravarti
VP & Chief Scientific Officer



Gianna Cioffi
VP Customer Relations & Sales



Dr. Krystle Reiss
Senior Research Scientist



Shannon Bush
Customer Support Manager



Sai Radha Mani Alla
Senior Software Developer

Special Thanks

We extend our sincere thanks to Neotel Systems and Services, our valued local distribution partner, for their support and efforts in organizing our Annual Meeting.



Event Schedule

9:00 – 9:55 AM

WELCOME TEA AND CHECK-IN

9:55 – 10:00 AM

INTRODUCTION

Manoranjan Singh Sidhu, *Neotel Systems and Services*

10:00 – 10:45 AM

MULTICASE PRESENTATION

Comprehensive *in silico* Toxicity Evaluations Using MultiCASE Tools

→ Presented by Dr. Suman Chakravarti

10:45 – 11:15 AM

GUEST SPEAKER

In silico (Q)SAR and E&L – Best Practices in Safety Assessment

→ Presented by Dr. Ravichandra BV, Amneal

11:15 – 11:35 AM

MULTICASE PRESENTATION

Exploring the MultiCASE Product Suite: From Data to Predictive Workflows

→ Presented by Sai Radha Mani Alla

Event Schedule

11:35 – 12:40 PM

LUNCH BREAK

12:45 – 1:30 PM

MULTICASE PRESENTATION

The Role of Metabolism on Complex Nitrosamines

→ *Presented by Dr. Suman Chakravarti*

1:30 – 2:00 PM

GUEST SPEAKER

NDSRI's Risk Assessment - QSAR Approach and Analytical Approach

→ *Presented by Dr. Amit Gosar, Indoco*

2:00 – 2:30 PM

GUEST SPEAKER

The Curious Case of Nitrosamines: Recalls, Misalignments, Gaps and the Emerging Trends

→ *Presented by Dr. Sushant Kamath, Abbott*

2:30 – 2:45 PM

TEA BREAK

Event Schedule

2:45 – 3:15 PM

MULTICASE PRESENTATION

Risk Assessment for Nitrosoureas: Contending with the Nitrosamine Extended Family

→ *Presented by Dr. Krystle Reiss*

3:15 – 3:35 PM

NEOTEL PRESENTATION

When Chemistry Meets Compliance: QSAR Models in ICH M7

→ *Presented by Yatindra Nath Yadav*

3:35 – 4:15 PM

PANEL DISCUSSION AND Q&A

Practical Challenges in Applying *In Silico* Methods

→ *All Speakers*

4:15 – 5:00 PM

FAREWELL SOCIAL

Tea and small plates will be served.

Thank you for being part of this year's MultiCASE (Q)SAR User Meeting. We appreciate your participation and hope to see you next year!

Expert Speakers



Dr. Suman Chakravarti | MultiCASE, Inc.



At MultiCASE, Suman is responsible for research and oversees product design and development, including converting ideas to viable products. He is the principal author of CASE Ultra, QSAR Flex, and META Ultra software. He has a master's and PhD in Medicinal and Pharmaceutical Chemistry, specializing in Computational Chemistry, QSAR, Cheminformatics, and Programming.



Dr. Ravichandra BV | Amneal



Dr. Ravichandra is a board-certified toxicologist (DABT, ERT) with over 17 years of experience in global drug development. He leads Global Toxicology & Nonclinical Development at Amneal Pharmaceuticals and has held roles at Elanco, Dr. Reddy's, Cipla, and Zydus.

His expertise includes toxicology, ADME, and pharmacology, with a focus on risk assessment, genotoxicity, nitrosamines, (Q)SAR, and extractables and leachables. He has supported IND, NDA, ANDA, and DMF submissions across discovery and generic programs.



Sai Radha Mani Alla | MultiCASE, Inc.



Sai Radha Mani Alla is a Software Developer at MultiCASE Inc., where she has contributed to product development for over seven years. She holds a master's degree in Computer Science from the University of Akron. Her work focuses on building and enhancing software features that streamline workflows and improve user experience. She plays a key role in developing core functionalities across MultiCASE products, including CASE Ultra and QSAR Flex. Working closely with internal teams, she translates practical challenges into intuitive solutions, helping users perform complex analyses more efficiently and effectively.

Expert Speakers



Dr. Amit Gosar | Indoco

Dr. Amit Gosar is a senior pharmaceutical leader with over 25 years of experience across research, quality, business development, and operations. He has led multidisciplinary teams of more than 120 scientists in chemical and analytical research, technology transfer, and contract analytical services for APIs, with expertise in extractables and leachables (E&L), IVBE studies, and genotoxicity assessments.

He has overseen analytical R&D and operations at a USFDA-approved laboratory at Indoco Remedies Ltd., contributed to over 70 publications, and holds two international patents. Dr. Gosar has received multiple industry awards for leadership and holds advanced degrees in chemical technology, chemistry, and clinical psychology, along with multiple doctorates and an MBA.



Dr. Sushant Kamath | Abbott

Dr. Sushant Kamath is a board-certified toxicologist and Senior Manager of Risk Assessment in the Global Preclinical & Product Safety division at Abbott Healthcare Pvt. Ltd. He focuses on toxicological risk assessment across product portfolios using AI/ML, QSAR, and read-across approaches, and supports the development of nonclinical safety studies for global registration of generic products.

He holds a PhD in Toxicology and has prior experience in BA/BE studies and in vitro DMPK. His work is driven by an interest in advancing New Approach Methodologies (NAMs) and AI-based models aligned with the 3Rs principles for animal-free testing.



Expert Speakers



Dr. Krystle Reiss | MultiCASE, Inc.

Krystle Reiss is a Senior Research Scientist at MultiCASE. She earned a Bachelor of Science in Chemistry and Mathematics from Alma College in Michigan before graduating from Yale University in 2021 with a PhD in Theoretical Chemistry. Her PhD work was focused on using computational methods to model proteins, bioinorganic systems, and drug binding, using both classical simulations and quantum mechanics calculations. After graduating, she worked as a computational chemist at Illumina, using ab initio calculations to predict and mitigate the photobleaching of fluorescent dyes used in DNA sequencing and expanding Illumina's computational chemistry capabilities. Krystle joined MultiCASE at the beginning of 2024 and has been working to build new statistical models to predict toxicological and degradation endpoints, as well as teaching new users how to use the software and interpret reports.



Yatindra Nath Yadav | Neotel Systems & Services

Yatindra Nath Yadav holds a Master's degree in Bioinformatics from the West Bengal University of Technology. He currently leads the Applications team in India for MultiCASE and also oversees sales and customer support functions. He works closely with pharmaceutical companies, research institutions, and CROs to support software implementation, technical workflows, and day-to-day user needs. His role combines application expertise, technical support, and client relationship management, making him a key point of contact for organizations using MultiCASE solutions.

