



## Compound Discoverer Training Bremen, Germany

9<sup>th</sup> December 2025

Goldener Saal | Atlantic Grand Hotel | Bremen, Germany

Responding to customer demand following the success of the training day at the 2024 Thermo Scientific™ Compound Discoverer™ software users meeting, we are excited to again offer an optional 1-day training before the 2-day user meeting.

During this training, you will learn the fundamentals of using Compound Discoverer and develop towards using more of the specialized tools available in the software – all guided by Thermo Fisher Scientific experts.

We look forward to welcoming you in Bremen!

### Agenda – Tuesday 9<sup>th</sup> December

8.45 am *Registration desk opens*

9:15 am **Welcome, introduction**

9:30 am **Session 1: How to get started for new users**

11:00 am *Coffee break*

11.30 am **Session 2: Untargeted applications e.g. Metabolomics/E&L/Environmental**

1:00 pm *Lunch*

2:00 pm **Session 3: MetID/Transformation/Environmental fate**

3:30 pm *Coffee break*

4:00 pm **Session 4: Specialized tools**

5:00 pm **Q&A & wrap up**

Register at [thermofisher.com/discoverersoftwareusermeeting](https://thermofisher.com/discoverersoftwareusermeeting)



# Compound Discoverer Users Meeting Bremen, Germany

10-11<sup>th</sup> December 2025

Goldener Saal | Atlantic Grand Hotel | Bremen, Germany

Join us at the 2025 Thermo Scientific™ Compound Discoverer™ Software Users meeting. For two days, you will learn from experts and connect with other users to further your path to success. Take the opportunity to discuss your workflows, tour our factory in Bremen, the home of the Thermo Scientific™ Orbitrap™ and Astral™ mass spectrometers and visit the Bremen Christmas market.

We look forward to welcoming you in Bremen!

## Agenda – Wednesday 10<sup>th</sup> December

8.45 am	Registration desk opens	
9:15 am	<b>Welcome, introduction</b>	Tim Stratton
9:30 am	<b>Recap of enhancements in Compound Discoverer 3.4 software</b>	Ralf Tautenhahn
10:30 am	<b>Introducing Compound Discoverer 3.5 software</b>	Ralf Tautenhahn
11:00 am	Coffee break	
11:30 am	<b>Extractables and Leachables testing by a CRO using Non-Targeted Analysis: Challenges and implementation use cases of Compound Discoverer software at Nelson Labs</b>	Phillipe Verlinde, Toxicon
12:00 pm	<b>Update on Spectral Libraries</b>	Tim Stratton
12:30 pm	Lunch	
1.30 pm	<b>New features in mzCloud™</b>	Marynka Ulaszewska
2.00 pm	<b>Metabolomic approach to support food safety in innovative milk processing: the case of infrared (IR) treatment</b>	Maria Nobile, Ph.D., Università degli Studi di Milano
2:30 pm	<b>Reporting compound annotation confidence using automated scoring</b>	Ralf Tautenhahn
3:00 pm	Coffee break	
3:30 pm	<b>Accessing Compound Discoverer Result Files using PyEDS</b>	Martin Strohm
4:00 pm	<b>How to create a scripting node</b>	Ralf Tautenhahn
4:30 pm	<b>Untargeted PFAS analysis in Compound Discoverer software</b>	Richard Cochran
5:00 pm	<b>User feedback and market insights</b>	Dave Abramowitz
7.30pm	Networking dinner at Canova Restaurant & Café in der Kunsthalle	

## Agenda – Thursday 11<sup>th</sup> December

9.00 am	<b>Discussion: Best practices for experiment design, acquisition &amp; processing</b>	All
10.00 am	<b>Identifying molecular structures with a SIRIUS node in Compound Discoverer software</b>	Lee Ferguson, Duke University, USA
10.30 am	Coffee break	
11.00 am	<b>Stable isotope labelling (targeted and untargeted)</b>	Ralf Tautenhahn
11:30 am	<b>Neutral loss search &amp; compound class scoring</b>	Tim Stratton
12.00 pm	<b>Molecular Networking</b>	Tim Stratton
12.30 pm	Lunch	
1.30 pm	<b>GC-HRMS workflows in Compound Discoverer software</b>	Nicholas Warner
2:00 pm	<b>Tips &amp; tricks: Import/export, table navigation, summaries, custom plots...</b>	Ralf Tautenhahn, Abhinandan Shrestha
2.30 pm	<b>Q&amp;A &amp; wrap up Day 2</b>	All
3.00 pm	<b>Optional: Factory tour (duration approx. 1.5hr) OR 1-2-1 discussions with experts</b>	Sign up on site

 Register at [thermofisher.com/discoverersoftwareusermeeting](https://thermofisher.com/discoverersoftwareusermeeting)