

# **Training Courses for Life Science Mass Spectrometry 2023**

On Instrumentation, Software Packages and Solutions

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# Power up Your Skills and Share Your Knowledge

Trainings on Bruker instrumentation, software packages and solutions are provided by very experienced application experts.

Various courses are available covering the range from absolute beginners to experienced users.

- Training
- Improvement
- Practice
- Focus
- Intelligence
- Lesson
- Motivation
- Success

# **General Remarks and Information for Training Courses**

### Registration

For registration, please access the online registration at www.bruker.com.

#### Confirmation

After receiving your registration form your participation will be confirmed. If the selected training course is already fully booked, an alternative date will be offered.

#### **Training costs**

Training costs include the course fees as well as lunch and beverages during the training.

Travel and accommodation are excluded.

Please contact your local Bruker Training Center to get a list of recommended hotels located nearby.

#### Cancellation

Bruker reserves the right to cancel the training if the minimum number of participants is not achieved one month prior to the training date. Please wait with your travel arrangements until receipt of confirmation.

Customers may cancel in writing not later than one month prior to the training date at a full refund of the training price. If customer cancels later than 2 weeks before the training, the full training fee will be charged. Customers may substitute a colleague without extra charge or payment in this case.

### **Course language**

All courses will be held in English unless otherwise explicitly stated or agreed between customer and Bruker trainer.

Bruker general terms and conditions of supply and service apply.

## **Overview**

# Training Courses at a Training Center

### **Essential Operator Training Courses**

- Introductory courses at a Bruker training center.
- Includes instrument control, data acquisition and processing.
- Includes sample preparation and application-specific training
- If HPLC is required, it includes application relevant HPLC aspects but does not substitute an explicit HPLC training.
- The number of participants is usually limited to 6 persons per course.
- Price is per person and excludes all travel and lodging expenses.

### **Advanced Operator Training Courses**

- Prerequisite for attending an advanced operator training course is the successful participation in an essential operator training course.
- Basic theory will be touched on, but will not be in the focus of advanced trainings.
- Comprehensive software courses to give an overview of software functionalities for a fast productivity ramp-up.
- Price is per person and excludes all travel and lodging expenses.

# Onsite Training Courses

### **Onsite Operator Training Courses**

- Contents are defined prior to the training between the customer and Bruker training center.
- Time needs should be calculated analogously to the factory training courses. Parameter optimization in your lab and of your instrument requires approximately an additional half day.
- The number of participants in the training is not limited but should not exceed a reasonable number to ensure a good interaction between trainees and trainer (usually up to 5 persons). A training room should be provided by the customer to ensure a productive training.
- Bruker reserves the right to convert an ordered onsite training into an in-house training in case of war, civil war, political instability, the risk of terrorist activity, pandemics or natural disasters which pose a significant threat for Bruker employees. In this case, Bruker will carry the costs for traveling in economy class to the Bruker training center providing the training as well as lodging costs for a maximum of two training participants. Travel costs of accompanying persons not participating in the training cannot be covered.

# Online Training Courses

### **Online Operator Training Courses**

- Software training courses are offered online to ensure your lab productivity efficiently.
- To offer trainings during times when travelling is difficult or not allowed a variety of online trainings is available.
- Courses can be spread on multiple sessions to allow for smaller amount of information per session.



# LabScape® Service & Lifecycle Support

# Maintenance Service Agreements for Life Science

	LabScape Connect	LabScape Essential	LabScape Access	LabScape Complete	LabScape Complete 48
Remote Services					
Remote Monitoring*	<u> </u>	<u> </u>	<u> </u>	<b>⊗</b>	<u> </u>
Unlimited Priority Remote Support	<b>Ø</b>	<b>Ø</b>	<b>Ø</b>	<b>S</b>	<b>Ø</b>
Software services					
Compass & Data Analysis SW Upgrades	<u> </u>	<u> </u>	<u> </u>	<u> </u>	<u> </u>
Postprocessing SW Licenses & Upgrades**		discount	discount	premium discount	premium discount
Upgrade of Postprocessing Software**				1 Voucher p.a	1 Voucher p.a
Regular Maintenance					
Regular Maintenance Work and Parts		<b>Ø</b>	<u> </u>	<b>Ø</b>	<u> </u>
Onsite Repair Services and Parts					
Unlimited Repair Visits incl. Spare Parts			<b>S</b>	<b>⊗</b>	<b>⊗</b>
Wear and Tear Part Replacement	discount	discount	discount	<b>Ø</b>	<b>Ø</b>
Loaner Equipment*					<b>Ø</b>
Compliance Services					
Operational Qualification / Perform. Validation					included
Onsite Response Service Level					
Onsite Response			3-5 business days	3-5 business days	2 <sup>nd</sup> business day
Additional benefits					
Consumable Parts	discount	discount	discount	premium discount	premium discount
Operation Training or Applications Training	discount	discount	discount	premium discount	premium discount

<sup>\*</sup> if applicable to the respective product

<sup>\*\*</sup> SCiLS™ Lab, MetaboScape®, BioPharma Compass®

# Training Center Contact Information

### Europe

### **Bruker Daltonics GmbH & Co. KG**

Fahrenheitstrasse 4 28359 Bremen, Germany Phone: +49 (421) 2205-1464 Fax: +49 (421) 2205-104 Email: Training-HB@Bruker.com

### **Bruker Daltonique S.A.**

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### **Bruker Española S.A**

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### America

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### **Bruker Scientific LLC**

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### Bruker do Brasil Ltda.

Condomínio BBP – Barão de Mauá Rod.D.Pedro I, km 87.5 (pista norte) 12954-260 Atibaia, SP, Brazil

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### Asia

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1-8-29, Nishimiyahara Yodogawa-ku Osaka-city Osaka 532-0004, Japan Phone: +81 (45) 4400478 Fax: +81 (45) 4532458

Email: Training.BDAL.JP@bruker.com Training course available in Japanese

language

# Bruker (Beijing) Scientific Technology Co., Ltd

8F, Tower C, Building B-6, No.66 Xi Xiao Kou Road, Haidian District Beijing 100192, China Phone: +86 (10) 5833 3000 Fax: +86 (10) 5833 3030 Email: MS\_Training\_China@bruker.com Training course is available in Chinese language

# Bruker (Shanghai) Scientific Technology Co., Ltd

Shanghai Office 9F, Building NO.1, Lane 2570, Hechuan Rd, Minhang District Shanghai 200233, China Phone: +86 21 51720800

Fax: +86 (021) 5172 0880

Email: MS\_Training\_China@bruker.com Training course is available in Chinese language

Language: Check language availability at your training center. In factory trainings are not available in some regions, please check with your training center.

# **Training Course Index**

All trainings provided (a training course from the list) with an instrument purchase can also be ordered as standalone trainings (please just look for the corresponding training order number).

Register Number	Training Name	Duration	Page
MALDI-TO	F Operator		
Essential C	perator Training Courses, In-House		
C1EP13	Proteomics	3 Days	13
C1EI12	MALDI Imaging	3 Days	14
C1ES13	Synthetic Chemistry and Polymers	3 Days	15
ESI-QTOF	Courses		
Essential C	perator Training Courses, In-House		
C3EL23	ESI-QTOF, Essential Operator Low Molecular Weight Applications	2.5 Days	17
C3EL33	ESI-QTOF, Essential Operator Training Course - Metabolomics	3 Days	18
C3EL43	ESI-QTOF, Essential Operator Training Course – TASQ®	3 Days	19
C3EP23	ESI-QTOF, Proteomics Applications	3 Days	20
C3EB13	ESI-QTOF, BioPharma Compass® Workflows	3 Days	21
C3ES13	ESI-QTOF, TargetScreener Solution	3 Days	22

Training Name	Duration	Page
ourses		
perator Training Courses, In-House		
timsTOF, Essential Operator Low Molecular Weight Applications	3 Days	24
timsTOF, Essential Operator Training Course – Metabolomics	3 Days	25
timsTOF, Essential Operator BioPharma Compass® Workflows	3 Days	26
timsTOF Pro, Essential Operator Proteomics Applications	3 Days	27
timsTOF SCP, Essential Operator Proteomics Applications	3 Days	28
ex Courses		
timsTOF fleX, Essential Operator MALDI Imaging	2 Days	30
perator Training Courses, In-House		
GC-MS TQ Essential Operator	3 Days	32
LC-MS TQ Essential Operator	3 Days	33
urses		
perator Training Courses, Onsite		
General	3 Days	35
MRMS, MALDI Imaging Application Course	2 Days	36
MRMS, Metabolomics Application Course	2 Days	37
MRMS, Petroleomics Application Course	2 Days	38
MRMS Riomolecules Application Course	2 Days	39
	timsTOF, Essential Operator Low Molecular Weight Applications  timsTOF, Essential Operator Training Course – Metabolomics  timsTOF, Essential Operator BioPharma Compass® Workflows  timsTOF Pro, Essential Operator Proteomics Applications  timsTOF SCP, Essential Operator Proteomics Applications  timsTOF SCP, Essential Operator Proteomics Applications  ex Courses  timsTOF fleX, Essential Operator MALDI Imaging  seperator Training Courses, In-House  GC-MS TQ Essential Operator  LC-MS TQ Essential Operator  urses  urses  perator Training Courses, Onsite  General  MRMS, MALDI Imaging Application Course  MRMS, Metabolomics Application Course	timsTOF, Essential Operator Training Courses, In-House timsTOF, Essential Operator Training Course – Metabolomics timsTOF, Essential Operator BioPharma Compass® Workflows timsTOF Pro, Essential Operator Proteomics Applications timsTOF Pro, Essential Operator Proteomics Applications timsTOF SCP, Essential Operator Proteomics Applications timsTOF SCP, Essential Operator Proteomics Applications  ex Courses timsTOF fleX, Essential Operator MALDI Imaging 2 Days  essential Operator 3 Days  perator Training Courses, In-House GC-MS TQ Essential Operator 3 Days  urses perator Training Courses, Onsite General 3 Days  MRMS, MALDI Imaging Application Course 2 Days  MRMS, Metabolomics Application Course 2 Days  MRMS, Petroleomics Application Course 2 Days

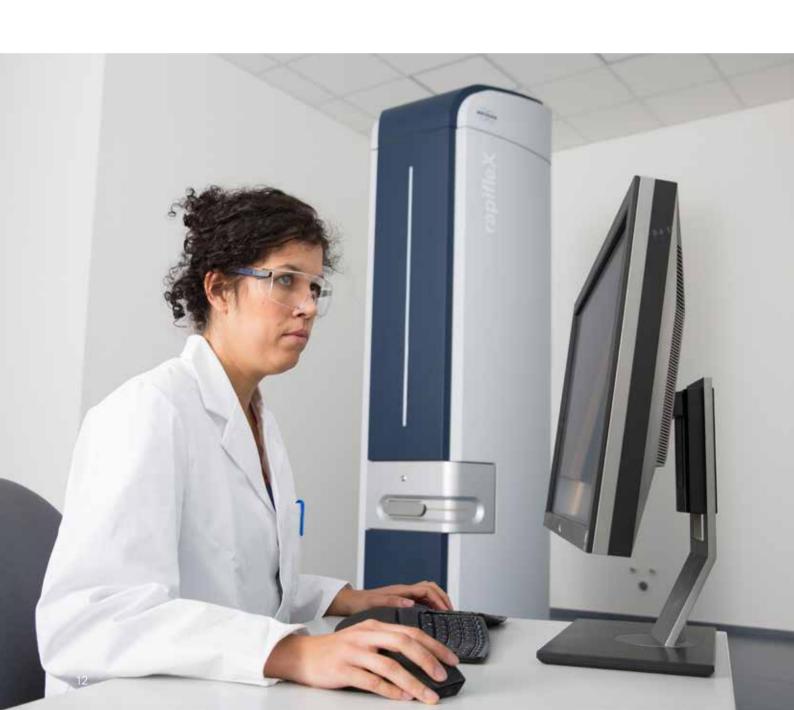
Register Number	Training Name	Duration	Page
ESI Ion Tra	ap Courses		
Essential C	perator Training Courses, In-House		
C2EL13	Low Molecular Weight Applications	2.5 Days	40
C2ET12	Toxtyper® Routine Workflows	3 Days	41
C2EP13	Proteomics	3 Days	42
Advanced	Operator Training Courses, In-House		
C2AA31	Peptide Analysis using ETD	1 Day	44
SPR Cours	ses		
Essential C	Operator Training Courses, In-House / Online		
D1EX01	SPR Pro Instruments	2 Days	46
D3AX01	SPR Individual Operator Onsite Training Course	up to 3 Days	47
Software	courses		
Advanced	Operator Training Courses, Online		
C9AA21	Statistical analysis of MALDI Imaging data using SCiLS™ Lab software	2 x 0.5 Days	49
C1AS11	Polymers and PolyTools	2 x 0.5 Days	50
C9AA21	MetaboScape®	2 x 0.5 Days	51
C9AA61	TASQ®	2 x 0.5 Days	52
C9AA32	BioPharma Compass®	2 x 0.5 Days	53
D2AX01	SPR Pro Instruments, Analyzer & Control Software	0.5 Days	54
Advanced	Operator Training Courses, Onsite		
C9AA61	General	2, 3, 4 or 5 Days	55

All essential or advanced operator trainings can also be ordered onsite. Online courses and 1 day training courses are exempted from this unless sold together with other onsite trainings.

# **MALDI-TOF Courses**

**Essential Operator Training Courses** 

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### **C1EP13**

# MALDI-TOF/TOF Essential Operator Training Course

## **Duration** 3 Davs

### **Proteomics**

### Links

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### Intention

This training course focuses on the basics of practical MALDI-TOF/TOF operation in the context of proteomics and protein analysis experiments. The course covers the essentials of sample preparation, data acquisition/processing and instrument maintenance, and, thus, will enable novice users getting started with MALDI-TOF/TOF analyses of peptides and proteins.

### **Prerequisite**

No deeper pre-experience is required. However, before attending the training course, participants are encouraged to take part in the user familiarization that is done at a customer site upon installation of the MALDITOF/TOF instrument, and to gain some first practical experience over a few weeks.

## Course Topics

#### Instrument overview

General introduction to the principles of MALDI-Compass® TOF(/TOF) (MALDI ionization, TOF(/TOF) analyzer).

### Sample preparation

Sample requirements (concentration, purity), sample pre-treatment (desalting), matrices of choice and matrix preparation protocols for various types of samples (peptides, proteins, incl. samples modified by e.g. phosphorylation, glycosylation).

### **Data acquisition**

Introduction to Bruker's flexControl software, optimization of most important acquisition method parameters (e.g. laser fluence, shot count per spectrum), automated data acquisition using autoXecute.

### **Data processing**

Introduction to Bruker's flexAnalysis software, peak annotation, smoothing, baseline subtraction, recalibation (internal / external), automated processing using flexAnalysis methods.

### **Data interpretation**

Introduction to Bruker's Biotools or BioPharma Compass® software, protein identification by database search (MASCOT), batchwise database searching using batch search methods.

### **Instrument maintenance**

Participants will be familiarized with all the maintenance operations that are to be done routinely by instrument users.

### **C1EI12**

# MALDI-TOF/TOF Essential Operator Training Course

# **Duration** 3 Days

## MALDI Imaging

### Links

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### Intention

This course is intended for beginners in the field of MALDI Imaging and will provide a comprehensive introduction to the entire workflow. The course is focused on the mass spectrometric analysis of tissue sections using Bruker MALDI-TOF hardware and software.

### **Prerequisite**

No detailed knowledge in mass spectrometry and / or histology is required to attend the course. Basic familiarity with Bruker MALDI-TOF instruments and a general understanding of the MALDI Imaging concept would be helpful. A substantial part of the course will be conducted in a level 2 biosafety lab.

## **Course Topics**

### Instrument overview

General introduction to the principles of MALDI-TOF/TOF (MALDI ionization, TOF(/TOF) analyzer).

Introduction to the concept of MALDI Imaging.

### Sample preparation

Requirements to sample materials, preparation of tissue sections on conductive slides, deposition of MALDI matrix.

MALDI-TOF instrument operation (basics) (Introduction to flexControl software, method setup for MALDI imaging analyses).

### **Data acquisition**

Acquisition of MALDI Imaging data using flexImaging software.

### **Consolidation training**

Deposition of MALDI matrix, acquisition of MALDI Imaging data using flexImaging software, batch acquisition of multiple MALDI Imaging datasets.

Visualization of MALDI Imaging data in flexImaging software.

Data reprocessing workflow.

### **C1ES13**

# MALDI-TOF/TOF Essential Operator Training Course

# **Duration** 3 Days

## Polymers and Synthetic Chemistry

### Links

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### Intention

This training course focuses on the basics of practical MALDI-TOF/TOF operation in the context of polymer and synthetic chemicals analysis. The course covers the essentials of sample preparation, data acquisition/processing and instrument maintenance, and, thus, will enable novice users getting started with MALDI-TOF/TOF analyses of synthetic polymers and further classes of organic and inorganic compounds.

### **Prerequisite**

No deeper MALDI-TOF/TOF pre-experience is required. However, before attending the training course, participants are encouraged to take part in the user familiarization that is done at a customer site upon installation of the MALDI-TOF/TOF instrument, and to gain some first practical experience over a few weeks.

## Course Topics

#### Instrument overview

General introduction to the principles of MALDI-TOF/TOF (MALDI ionization, TOF(/ TOF) analyzer).

### Sample preparation

Sample requirements (concentration, purity), matrices of choice and matrix preparation protocols for various types of samples (in particular: synthetic polymers, further compound classes will be treated on demand).

### **Data acquisition**

Introduction to Bruker's flexControl software, optimization of most important acquisition method parameters (i.e. laser fluence, shot count per spectrum).

### **Data processing**

Introduction to Bruker's flexAnalysis software, peak annotation, smoothing, baseline subtraction, recalibration (internal/external), automated processing using flexAnalysis methods.

### **Data interpretation**

Introduction to Bruker's PolyTools software, determination of end groups, number-average molar mass  $\rm M_{_{\rm N}}$ , mass-average molar mass  $\rm M_{_{\rm W}}$  and dispersity of synthetic polymer samples

### Instrument maintenance

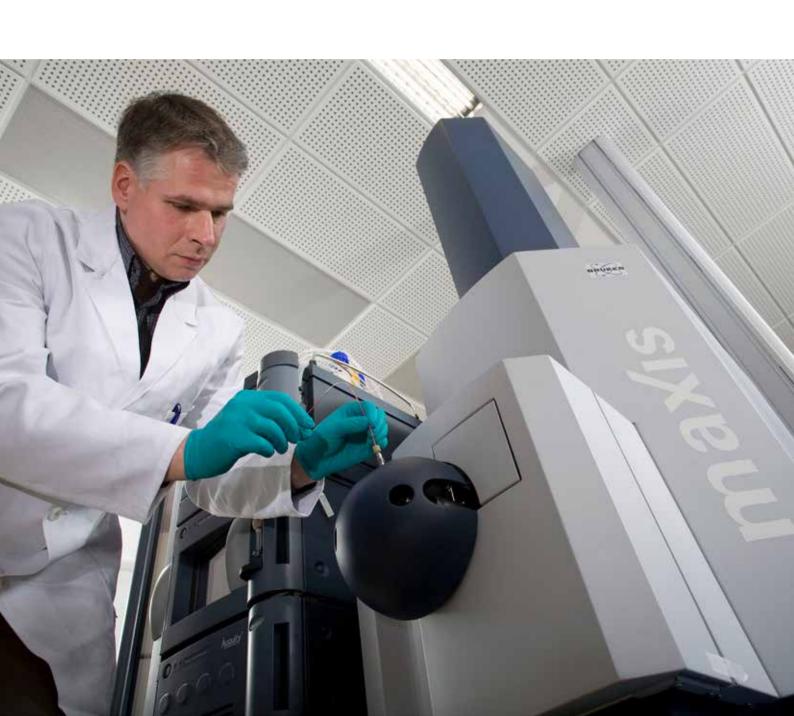
Participants will be familiarized with all the maintenance operations that are to be done routinely by instrument users.

# **ESI-QTOF Operator**

Training courses cover the range from instrument control to application driven solution

**Essential Operator Training Courses** 

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### **C3EL23**

# **ESI-QTOF Essential Operator Training Course**

# **Duration** 2.5 Days

# ESI-QTOF, Low Molecular Weight Applications

### Links

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### Intention

This course is intended for novice Bruker QTOF users without significant prior experience in data acquisition, data processing and instrument maintenance. The course covers all important aspects of QTOF operation, including application-relevant HPLC aspects, but it does not substitute a dedicated HPLC training. The post processing of the data is done with the DataAnalysis software. To include MetaboScape® or TASQ® choose courses C3EL33 or C3EL43, respectively.

### **Prerequisite**

Due to the familiarization during the system installation, participants should have a basic knowledge of the QTOF mass spectrometer (compact, impact, maXis) and some initial experience with the hardware and the software.

Please note: This training does not replace a dedicated HPLC training!

### Course Topics

### **Introduction to Bruker QTOF systems**

Overview over hardware and software. System components and function. Highresolution MS and MS/MS acquisition modes.

### **Atmospheric pressure ionization (API)**

Fundamentals of electrospray ionization (ESI). Requirements regarding solvent and buffers, default settings for the ESI source. Basics of APCI, APPI and VIP-HESI, if applicable.

# Calibration and tuning of the instrument

Introduction to otofControl software. Mass calibration and tuning of the instrument. Explanation of source and tune parameters. Methods for small molecule analysis.

### MS/MS modes and parameters

Applications for different MS/MS modes: Data dependent MS/MS, MRM and bbCID. Parameters for intelligent precursor selection in autoMS/MS mode. In-source CID and pseudo MS<sup>3</sup>.

### **HPLC-MS** analysis

Introduction to the HyStar software. Set-up of HPLC methods and preparation of sample tables. Acquisition of LC-MS/MS data.

#### Data analysis

Overview over the DataAnalysis software. General data processing: Recalibration of data, generation of extracted ion chromatograms (EICs), extraction of MS and MS/MS spectra, calculation of elemental compositions (SmartFormula). Advanced features: Different algorithms for feature extraction, CompoundCrawler, FragmentationExplorer, LibraryEditor.

### **Maintenance**

Guidelines and recommendations for the maintenance of the QTOF instrument. Ion source cleaning.

### **Applications**

Application-specific questions are discussed upon request.

### **C3EL33**

# **ESI-QTOF Essential Operator Training Course - Metabolomics**

# **Duration** 3 Days

# ESI-QTOF, Low Molecular Weight Applications including MetaboScape

### Links

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### Intention

The course is intended for novice Bruker QTOF users without significant prior experience in data acquisition and / or instrument maintenance. The course covers all important aspects of QTOF operation as well as application-relevant HPLC aspects but does not substitute an explicit HPLC training. It includes a 0.5 day basic training of MetaboScape software for data processing, annotation of unknown compounds, and statistical analysis.

### **Prerequisite**

Due to the familiarization during system installation, attendees should have a basic knowledge of the QTOF mass spectrometer (compact, impact, maXis) with several weeks of experience with the instrument and the software. Basic knowledge about statistics is of advantage.

Please note: This training does not replace a dedicated HPLC training!

### **Course Topics**

#### Instrument overview

Instrument geometry, theory of the orthogonal time of flight system, accurate mass measurement, MS/MS capabilities of the instrument.

### **Atmospheric pressure ionization (API)**

ESI, APCI, APPI, VIP-HESI, ionization efficiency, positive and negative ion mode ionization, direct infusion, electrolyte and buffer requirements for MS coupling of HPLC and UHPLC.

## Tuning and optimization of the instrument

Calibration and tuning of the instrument, ion transfer, tuning for high sensitivity and high mass accuracy, resolution, mass range and mass accuracy.

### **Data acquisition**

Data acquisition speed depending on sample complexity, HPLC control using HyStar software. Introduction to Metabolomics studies.

### MS/MS capabilities

Isolation, fragmentation, auto MS/MS, MRM, intelligent precursor selection, In-source fragmentation, pseudo MS<sup>3</sup>, broadband CID.

### **Data Analysis**

General data processing and evaluation using DataAnalysis, SmartFormula, basic introduction to the LibraryEditor and ReportDesigner. Introduction to statistical data mining: PCA, t-Test, ANOVA and others. Data handling in MetaboScape, feature extraction, optimizing processing parameters. Discussion about statistical models in MetaboScape for different analytical questions.

### **Metabolite Identification**

Identification of compounds with SmartFormula (exact mass, isotopic pattern), retention times and MS/MS spectra by using AQ scoring. Search strategies using additional annotation tools in MetaboScape, such as Target Lists, and MS/MS spectra libraries (e.g. HMDB, MetaboBase and personal libraries). Structure elucidation with database searches (e.g. ChemSpider) and in-silico fragmentation.

#### **Maintenance**

General maintenance of the QTOF, source maintenance, including dismantling and methods of cleaning.

### **C3EL43**

# **ESI-QTOF Essential Operator Training Course - TASQ®**

# **Duration** 3 Days

# ESI-QTOF, Low Molecular Weight Applications including TASQ®

### Links

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### Intention

The course is intended for novice Bruker QTOF users without significant prior experience in data acquisition, data processing and instrument maintenance. The course covers all important aspects of QTOF operation including application relevant HPLC aspects, but it does not substitute a dedicated HPLC training. It includes a 0.5-day basic training of the TASQ® software for targeted screening and quantification.

### **Prerequisite**

Due to the familiarization during the system installation, participants should have a basic knowledge of the QTOF mass spectrometer (compact, impact, maXis) and some initial experience with the hardware and the software.

Please note: This training does not replace a dedicated HPLC training!

### Course Topics

### **Introduction to Bruker QTOF systems**

Overview over hardware and software. System components and function. Highresolution MS and MS/MS acquisition modes.

### **Atmospheric pressure ionization (API)**

Fundamentals of electrospray ionization (ESI). Requirements regarding solvent and buffers, default settings for the ESI source. Basics of APCI, APPI and VIP-HESI, if applicable.

# Calibration and tuning of the instrument

Introduction to otofControl software. Mass calibration and tuning of the instrument. Explanation of source and tune parameters. Methods for small molecule analysis.

### MS/MS modes and parameters

Applications for different MS/MS modes: Data dependent MS/MS, MRM and bbCID. Parameters for intelligent precursor selection in autoMS/MS mode. In-source CID and pseudo MS<sup>3</sup>.

### **HPLC-MS** analysis

Introduction to the HyStar software. Set-up of HPLC methods and preparation of sample tables. Acquisition of LC-MS/MS data.

### **Data analysis**

Overview over the DataAnalysis software. General data processing: recalibration of data, generation of extracted ion chromatograms (EICs), extraction of MS and MS/MS spectra, calculation of elemental compositions (SmartFormula).

### Screening and quantitation in TASQ®

Execution of screening and quantitation workflows in TASQ®: batch import, TASQ® method parameters, data review, screening and quantitation workflow.

### **Maintenance**

Guidelines and recommendations for the maintenance of the QTOF instrument. Ion source cleaning.

### **C3EP23**

# **ESI-QTOF Essential Operator Training Course**

# **Duration** 3 Days

## ESI-QTOF, Proteomics Applications

#### Links

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### Intention

This course is intended for novice Bruker QTOF users without significant prior experience in data acquisition and / or instrument maintenance. This course covers all important aspects of maXis system operation as well as application relevant HPLC aspects but does not substitute an explicit HPLC training.

### **Prerequisite**

Due to the familiarization during system installation, attendees should have a basic knowledge of the ESI-QTOF mass spectrometer with several weeks of experience with the instrument and the software.

Please note: This training does not replace a dedicated HPLC training!

### **Course Topics**

### Instrument overview

Instrument geometry, theory of the Bruker QTOF systems, accurate mass, MS<sup>2</sup>-capabilities.

### **Data acquisition**

Resolution, calibration. HPLC control using HyStar software.

### Tuning and optimization of the maXis

Calibration and tuning of the QTOF system, ionization mode, ion transfer, tuning for high sensitivity/high resolution or wide mass range.

### **MS/MS-experiments**

Isolation, fragmentation, Auto-MS<sup>2</sup>, MRM experiments, intelligent precursor ion selection.

### **Atmospheric pressure ionization (API)**

ESI operation, ionization efficiency, direct infusion, coupling to high and low flow separation instruments (UHPLC and nanoLC).

### **Data analysis**

General data processing, accurate mass, recalibration, deconvolution (including MaxEnt), peaklist generation and export.

### **Database searching**

File export options, basics of BioTools and BioPharma Compass® software, database search.

#### **General maintenance**

Source maintenance, including dismantling and methods of cleaning.

### **Applications**

Specific requirements of the customer with respect to the focus of this course will be discussed.

### **C3EB13**

# **ESI-QTOF Essential Operator Training Course**

# **Duration** 3 Days

## ESI-QTOF, BioPharma Compass Workflows

### Links

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### Intention

This course is intended for novice users of the Bruker QTOF equipment combined with the software suite BioPharma Compass® without significant prior experience in data acquisition and processing. This course covers all important aspects of QTOF operation and (automated) workflow-based processing with BioPharma Compass® as well as application relevant HPLC aspects but does not substitute an explicit HPLC training.

### **Prerequisite**

Course participants should have attended the system and software familiarization during instrument and BioPharma Compass server installation and a few weeks of instrument and software use to develop some basic experience with the necessary hardware and software setup.

### Course Topics

### Instrument overview

Instrument geometry, theory of the orthogonal time of flight system, accurate mass measurement, MS/MS capabilities of the instrument.

### **Atmospheric pressure ionization (API)**

ESI ionization efficiency, direct infusion, electrolyte and buffer requirements for MS coupling of separation instruments like HPLC or UHPLC.

### Tuning and maintenance of the QTOF

Calibration and tuning of the QTOF, general maintenance of the QTOF, source maintenance, including dismantling and methods of cleaning.

### **Data acquisition**

Setup and method optimization options for measurements of intact protein and peptide mapping samples.

### **Data analysis**

General data processing and evaluation using DataAnalysis software.

### **BioPharma Compass introduction**

Introduction to BioPharma Compass functionalities and introduction to the supported workflows.

### **Administrative tasks**

Basic administrative tasks are shown for BioPharma Compass software suite including user-, station-, workflow- and method management.

#### **Automation**

BioPharma Compass is a turnkey solution, meaning that the whole process of acquiring data, analysis of data, report generation and result storage can be executed without the need of user intervention. The workflow and method concept is discussed, samples will be submitted, measured and analyzed. Available tools for inspecting results are shown.

### Reprocessing and validation

The functionality for reprocessing of acquired data sets and validation of obtained results are discussed.

### Workflows in detail

Details of the workflows protein screening, top-down ESI, peptide mapping, peptide mapping/PTM comparison, peptide screening, peptide screening/batch comparison are presented and discussed.

### **C3ES13**

# **ESI-QTOF Essential Operator Training Course**

# **Duration** 3 Days

# ESI-QTOF, TargetScreener HR Solution, Workflow Training

### Links

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### Intention

This course is intended for novice users of the Bruker TargetScreener solution without significant prior experience in data acquisition, data processing and instrument maintenance. The course covers all important aspects of the Bruker TargetScreener solution including application relevant HPLC aspects, but it does not substitute a dedicated HPLC training.

### **Prerequisite**

Due to the familiarization during the system installation, participants should have basic knowledge of the TargetScreener solution.

Please note: This training does not replace a dedicated HPLC training!

### Course Topics

### **Introduction to Bruker QTOF systems**

Overview over hardware and software. System components and function. Highresolution MS and MS/MS acquisition modes.

### Atmospheric pressure ionization (API)

Fundamentals of electrospray ionization (ESI). TargetScreener eluent composition for positive and negative ionization mode.

## Calibration and tuning of the instrument

Introduction to otofControl software. Mass calibration and tuning of the instrument. Explanation of source and tune parameters of the TargetScreener default methods.

### MS/MS modes and parameters

Use of broadband CID (bbCID) acquisition mode for screening and quantification and data dependent MS/MS for the extension of the TargetScreener database.

### **HPLC-MS** analysis

Introduction to the HyStar software. TargetScreener HPLC methods and preparation of sample tables. Acquisition of LC-MS/MS data.

### **Data analysis**

General data processing in DataAnalysis: Recalibration of data, generation of extracted ion chromatograms (EICs), extraction of MS and MS/MS spectra, calculation of elemental compositions (SmartFormula).

### Screening and quantitation in TASQ®

Execution of screening and quantitation workflows in TASQ®: batch import and management, TargetScreener method parameters, customization of TASQ® methods, data review, screening and quantitation workflow.

#### **Maintenance**

Guidelines and recommendations for the maintenance of the QTOF instrument. Ion source cleaning.

# timsTOF Operator

Training courses cover the range from instrument control to application driven solution

**Essential Operator Training Courses** 

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### **C8EL23**

# timsTOF Essential Operator Training Course

# **Duration** 3 Days

# timsTOF, Low Molecular Weight Applications

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### Intention

The course is intended for novice Bruker timsTOF users without significant prior experience in data acquisition and / or instrument maintenance. The course covers all important aspects of timsTOF operation as well as application relevant HPLC aspects but does not substitute an explicit HPLC training. To include MetaboScape® or TASQ® choose courses C8EL33 or C8EL43, respectively.

### **Prerequisite**

Due to the familiarization during system installation, attendees should have a basic knowledge of the timsTOF mass spectrometer with several weeks of experience with the instrument and the software.

### **Course Topics**

### Instrument overview

Instrument geometry, theory of the timsorthogonal time of flight system, accurate mass measurement, MS/MS capabilities of the instrument, introduction to ion mobility separation with tims technology.

### **Atmospheric pressure ionization (API)**

ESI, APCI, APPI, ionization efficiency, positive and negative ion mode ionization, direct infusion, electrolyte and buffer requirements for MS coupling of HPLC and UHPLC.

# Tuning and optimization of the instrument

Calibration and tuning of the instrument, ion transfer, tuning for high sensitivity and high mass accuracy, cycle and trigger times, resolution, mass range and mass accuracy, tuning of ion mobility for different resolution modes.

### **Data acquisition**

Data acquisition speed depending on sample complexity, HPLC control using HyStar software, strategies for acquiring data with and without ion mobility.

### MS/MS capabilities

Isolation, fragmentation, data dependent MS/MS, MRM, intelligent precursor selection, In-source fragmentation, pseudo MS³, broad band CID.

### **Data analysis**

General data processing and evaluation with DataAnalysis, SmartFormula and quantitation using QuantAnalysis software, basic introduction to the LibraryEditor and ReportDesigner. Heatmap of ion mobility data, extraction of relevant data out of ion mobility datasets, calculation of ion mobility resolution and CCS values.

### **Maintenance**

General maintenance of the timsTOF, source maintenance, including dismantling and methods of cleaning.

### **C8EL33**

# timsTOF Essential Operator Training Course

# **Duration** 3 Days

# timsTOF, Low Molecular Weight Applications including MetaboScape

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### Intention

The course is intended for novice Bruker timsTOF users without significant prior experience in data acquisition and / or instrument maintenance. The course covers all important aspects of timsTOF operation as well as application relevant HPLC aspects but does not substitute an explicit HPLC training. It includes a 0.5 day basic training of MetaboScape software for data processing, annotation of unknown compounds, and statistical analysis.

### **Prerequisite**

Due to the familiarization during system installation, attendees should have a basic knowledge of the QTOF mass spectrometer (compact, impact, maXis) with several weeks of experience with the instrument and the software. Basic knowledge about statistics is of advantage.

Please note: This training does not replace a dedicated HPLC training!

### **Course Topics**

#### Instrument overview

Instrument geometry, theory of the orthogonal time of flight system, accurate mass measurement, MS/MS capabilities of the instrument.

### **Atmospheric pressure ionization (API)**

ESI, APCI, APPI, ionization efficiency, positive and negative ion mode ionization, direct infusion, electrolyte and buffer requirements for MS coupling of HPLC and UHPLC.

# Tuning and optimization of the instrument

Calibration and tuning of the instrument, ion transfer, tuning for high sensitivity and high mass accuracy, resolution, mass range and mass accuracy.

### **Data acquisition**

Data acquisition speed depending on sample complexity, HPLC control using HyStar software. Introduction to Metabolomics studies.

### MS/MS capabilities

Isolation, fragmentation, Auto MS/MS, MRM, intelligent precursor selection, In-source fragmentation, pseudo MS³, broad band CID.

### **Data analysis**

General data processing and evaluation using DataAnalysis, SmartFormula, quantitation using QuantAnalysis software, basic introduction to the LibraryEditor and ReportDesigner. Introduction to statistical data mining: PCA, t-Test, ANOVA and others. Data handling in MetaboScape, feature extraction, optimizing processing parameters. Discussion about statistical models in MetaboScape for different analytical questions.

### Metabolite identification

Identification of compounds with SmartFormula (exact mass, isotopic pattern), retention times and MS/MS spectra by using AQ scoring. Search strategies using additional annotation tools in MetaboScape, such as Target Lists, and MS/MS spectra libraries (e.g. HMDB, MetaboBase and personal libraries). Structure elucidation with database searches (e.g. ChemSpider) and insilico fragmentation.

### **Maintenance**

General maintenance of the timsTOF, source maintenance, including dismantling and methods of cleaning.

### **C8EB13**

# timsTOF Essential Operator Training Course

# **Duration** 3 Days

### timsTOF, BioPharma Compass Software

### Links

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### Intention

This course is intended for novice users of the Bruker timsTOF instruments combined with the software suite BioPharma Compass® without significant prior experience in data acquisition and processing. This course covers all important aspects of instrument operation and (automated) workflow-based processing with BioPharma Compass as well as application relevant HPLC aspects but does not substitute an explicit HPLC training.

### **Prerequisite**

Course participants should have attended the system and software familiarization during instrument and had a few weeks of instrument and software use to develop some basic experience with the necessary hardware and software setup.

Please note: This training does not replace a dedicated HPLC training!

### Course Topics

### Instrument overview

Instrument geometry, theory of the orthogonal time of flight system, accurate mass measurement, MS/MS capabilities of the instrument.

### **Atmospheric pressure ionization (API)**

ESI ionization efficiency, direct infusion, electrolyte and buffer requirements for MS coupling of separation instruments like HPLC or UHPLC.

## Tuning and optimization of the instrument

Calibration and tuning of the instrument, ion transfer, tuning for high sensitivity and high mass accuracy, resolution, mass range and mass accuracy.

### **Data acquisition**

Setup and method optimization options for measurements of intact protein and peptide mapping samples.

### **Data analysis**

General data processing and evaluation using DataAnalysis software.

### **BioPharma Compass**

Introduction to BioPharma Compass functionalities and introduction to the supported workflows.

### **Administrative tasks**

Basic administrative tasks are shown for BioPharma Compass software suite including the management of users, stations, workflows and methods.

### **Automation**

BioPharma Compass is a turnkey solution, meaning that the whole process of acquiring data, analysis of data, report generation and result storage can be executed without the need of user intervention. The workflow and method concept is discussed, samples will be submitted, measured and analyzed. Available tools for inspecting results are shown.

### Reprocessing and validation

The functionality for reprocessing of acquired data sets and validation of obtained results are discussed.

### Workflows in detail

Details of the workflows protein screening, top-down ESI, peptide mapping, peptide mapping/PTM comparison, peptide screening, peptide screening/batch comparison are presented and discussed.

### **C8EP23**

# timsTOF Essential Operator Training Course

# **Duration** 3 Days

timsTOF, Proteomics Applications

### Links

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### Intention

The course is intended for novice Bruker timsTOF users without significant prior experience in data acquisition and / or instrument maintenance. The course covers all important aspects of timsTOF Pro operation as well as all application relevant HPLC aspects.

### **Prerequisite**

Due to the familiarization during system installation, attendees should have a basic knowledge of the timsTOF Pro mass spectrometer and LC set-up.

### Course Topics

### Instrument overview

Instrument geometry including the principle of ion mobility separation with tims and the time-of-flight (TOF) system. Introduction to different PASEF scan modes.

### **Captive spray**

Practical aspects of using the captive spray source for nanoflow applications.

## Tuning and optimization of the instrument

TIMS and TOF calibration. PASEF method parameter optimization using timsControl.

### **Data acquisition**

HPLC control using HyStar software. Optimization of methods for shotgun proteomics using timsControl software:

- General overview over MS and MS/MS parameters including different MS/MS capabilities, e.g. data dependent PASEF, data independent PASEF and parallel reaction monitoring PASEF
- Adjustment of MS and MS/MS relevant parameters according to sample complexity and aim of the analysis

### **Data analysis**

Manual inspection of acquired data in DataAnalysis, including heatmap of ion mobility data. Processing of proteomics datasets, preparation for database searches, and label free quantitation workflows.

#### Maintenance

General maintenance of the timsTOF, source maintenance and exchange, including dismantling and cleaning.

General nanoElute maintenance and troubleshooting.

### **C8EP33**

# timsTOF SCP Essential Operator Training Course

# **Duration** 3 Days

## timsTOF SCP, Proteomics Applications

### Links

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### Intention

The course is intended for novice Bruker timsTOF SCP users without significant prior experience in data acquisition and / or instrument maintenance. The course covers all important aspects of timsTOF SCP operation as well as all application relevant HPLC aspects, either with Bruker nanoElute or Evosep One.

### **Prerequisite**

Due to the familiarization during system installation, attendees should have a basic knowledge of the timsTOF SCP mass spectrometer and LC set-up.

### Course Topics

### Instrument overview

Instrument geometry including the principle of ion mobility separation with tims and the time-of-flight system. Introduction to different PASEF scan modes.

### **Captive spray**

Practical aspects of using the captive spray source for nanoflow applications.

## Tuning and optimization of the instrument

TIMS and TOF calibration. PASEF method parameter optimization using timsControl.

### **Data acquisition**

HPLC control using HyStar software, optimization of methods for shotgun proteomics timsControl software:

- General overview over MS and MS/MS parameters including different MS/MS capabilities, e.g. data dependent PASEF, data independent PASEF and parallel reaction monitoring PASEF
- Adjustment of MS and MS/MS relevant parameters according to sample complexity and aim of the analysis

### **Data analysis**

Manual inspection of acquired data in Data-Analysis: heatmap of ion mobility data.

Processing of proteomics data sets, preparation for data base searches, and label free quantitation workflows.

### **Maintenance**

General maintenance of the timsTOF SCP, source maintenance and exchange, including dismantling and cleaning.

General nanoElute or Evosep One maintenance and troubleshooting.

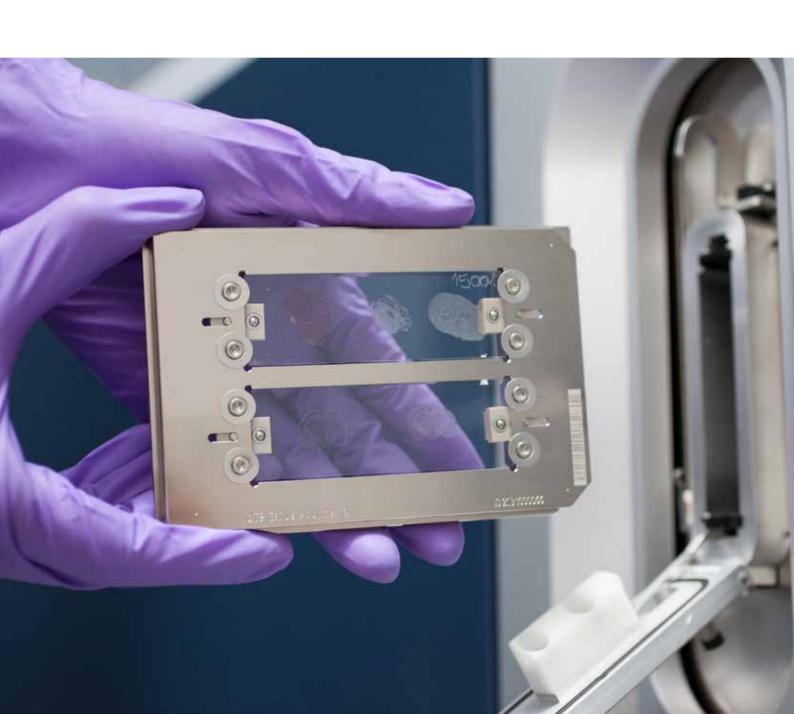
General discussion about handling low abundant samples.

# timsTOF fleX Operator

Training courses cover the range from instrument control to application driven solution

**Essential Operator Training Courses** 

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### **C8EI12**

# **Essential Operator MALDI Imaging Training Course**

# **Duration** 2 Days

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### Intention

This course is intended for beginners in the field of MALDI Imaging and will provide a comprehensive introduction to the entire workflow. The course is focused on the mass spectrometric analysis of tissue sections using the Bruker timsTOF fleX hardware and software.

### **Prerequisite**

Any detailed knowledge in mass spectrometry and / or histology is required to attend the course. Basic familiarity with Bruker's MALDI instruments and a general understanding of the MALDI Imaging concept would be helpful. A substantial part of the course will be conducted in a level 2 biosafety lab (factory course).

### **Course Topics**

### Introduction

Introduction to MALDI mass spectrometry. Concepts of MALDI Imaging and the MALDI Imaging workflow.

### Sample preparation

Sample preparation considerations regarding requirements to transportation and storage of good quality tissue samples. Cryosectioning: Introduction and hands-on training.

### **Matrix deposition**

Matrix selection guidelines, basics of HTX TM-sprayer instrument operation.

### Instrumentation

MALDI timsTOF flex instrument operation (TIMS off). Basics of timsControl software, method optimization for MALDI Imaging, calibration. Hands-on training for HTX TM-sprayer, including troubleshooting and method development guidelines. MALDI timsTOF flex instrument operation (TIMS on): Adjustment of timsControl software methods with TIMS on, method optimization for MALDI Imaging, calibration.

### Image acquisition

Introduction to flexImaging software and automatic image data acquisition. flexImaging software training: guided tour of all program features, including hands-on training.

### **Automation**

Batch acquisition of multiple MALDI images.

# **TQ Operator**

Training courses cover the range from instrument control to application driven solution

**Essential Operator Training Courses** 

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### **C6EA13**

# **GC-MS TQ Essential Operator Training Course**

# **Duration** 2 Days

### Links

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### Intention

This course is intended for novice Bruker EVOQ GC-MS Triple Quadrupole series users without significant prior experience in data acquisition and / or instrument maintenance. This course covers all important aspects of EVOQ TQ operation as well as application relevant GC aspects but does not substitute an explicit GC training.

### **Prerequisite**

Due to the familiarization during system installation, attendees should have a basic knowledge of the triple quad mass spectrometer with some experience with the instrument and the software.

Please note: This training does not replace a dedicated GC training!

### **Course Topics**

### Instrument overview

Instrument overview, GC-injectors, injection methods, theory of the quadrupol systems, different scan modes.

### **Electron impact ionization (EI)**

Principle of ion formation, ionization efficiency, in source fragmentation.

### **Chemical ionization (CI)**

Principle of ion formation, ionization efficiency, gases used for ionization, positive and negative ion mode ionization, requirements for laboratory.

## Advanced inlet techniques (on request)

Headspace Injection, ChromatoProbe.

### **Data acquisition**

Usage of System Control, Method Builder, tuning of the instrument: mass calibration and detector calibration, performance check/troubleshooting after tuning, ionization modes, scan-time, fragmentation in Q2.

### MS/MS capabilities

Isolation, fragmentation, MS/MS-method development, Compound Based Scanning.

### **Data analysis**

Introduction to tqControl-Software: general data processing in MSWS, using sequences, reprocessing and reports, advanced automated and manual integration for quantitative analysis.

### **Maintenance**

General maintenance of the GC and the mass spectrometer, source maintenance, including dismantling and methods of cleaning.

### **Applications**

Specific requirements of the customer with respect to the focus of this course will be discussed.

### **C7EA13**

# **LC-MS TQ Essential Operator Training Course**

# **Duration** 3 Days

### Links

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### Intention

This course is intended for novice Bruker EVOQ LC-MS Triple Quadrupole series (EVOQ Qube, EVOQ Elite, EVOQ Elite ER) users without significant prior experience in data acquisition and / or instrument maintenance. This course covers all important aspects of EVOQ TQ operation as well as application relevant LC aspects but does not substitute an explicit LC training.

### **Prerequisite**

Due to the familiarization during system installation, attendees should have a basic knowledge of the triple quad mass spectrometer with several weeks of experience with the instrument and the software.

Please note: This training does not replace a dedicated HPLC training!

### Course Topics

### Instrument overview

Familiarization with the LC-MS TQ system, theory of the quadrupol systems, different scan modes.

### Atmospheric pressure ionization (API)

Electrospray Ionization (ESI) and Atmospheric Pressure Chemical Ionization (APCI) operation, ionization efficiency, heated ESI characteristics.

### **Calibration and tuning**

Tuning of the instrument: mass calibration and detector calibration.

### Method handling and data acquisition

Instrument control, using MSWS and HyStar, creation and running of methods. Set-up and accomplishment of LC-MS/MS analyses.

### MS/MS-capabilities

Isolation, fragmentation, MS/MS-method development, Compound Based Scanning.

# Data analysis including efficient reporting

Introduction to MSWS-Software: general data processing in MSWS, using sequences, reprocessing and reports, advanced automated and manual integration for quantitative analysis.

Efficient reporting by DASH reporting.

#### **Maintenance**

Good working conditions (solvents, containers, nitrogen etc.), cleaning of the ion source, changing probes and capillaries.

### **Applications**

Individual questions and specific requirements with respect to the focus of this course will be discussed.

# **MRMS Operator**

Training courses cover the range from instrument control to application driven solution

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### **S4AA03**

# MRMS Operator Onsite Training Course

# **Duration** 3 Days

### General

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### Intention

This course is the basic training course for operation of the MRMS instrument. Additionally, to the basic instrument handling specific individual needs of our customers will be considered. The course will be held onsite at the customer using his installed instrumentation. This ensures that all applications trained during the course will for sure be applicable on the local installation.

### **Prerequisite**

Prerequisites depend on the actual training course content and should be discussed with the responsible application specialist from Bruker in advance of the training.

## **Course Topics**

- Basic operation of the MRMS instrument
- ftmsControl (instrument control software)
- MS method handling
- Instrument tuning for low, medium and high m/z ranges
- ParaCell™ shimming
- Positive and negative ion mode
- Fragmentation methods: FSD-CID, QCID, ETD and ECD
- ESI and MALDI mesurements of standard compounds
- Familiarization of software: HyStar, DataAnalysis and flexImaging

## S4AA02 C4EI15

# solariX and scimaX series MRMS MALDI Imaging Application Course

# **Duration** 2 Days

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### Intention

This training course is intended for novice Bruker solariX or scimaX series users without significant prior experience in MALDI Imaging experiments. Slide preparation, data acquisition, data analysis and instrument handling are included. The course covers all important aspects of data acquisition and data analysis for MALDI Imaging applications.

### **Prerequisite**

A MRMS Essential Operator Training Course should be passed before attending a MALDI Imaging training course.

### Location

Please check with your local Bruker Office where the training courses are offered.

### **Course Topics**

### Introduction

Theory of MALDI Imaging on the solariX or scimaX instrument series.

### Sample preparation

Standard tissue cutting on cryotome, application of matrix using the HTX TM sprayer, application of standards.

### **Calibration and tuning**

Mass calibration, tuning of ion transfer and ICR cell with special focus on analytes of interest (lipids/metabolites/peptides).

### MS operation

flexImaging and ftmsControl familiarization, mass resolution, speed, scan range, quadrupole isolation.

### Method handling and data acquisition

Method handling in ftmsControl and DataAnalysis. Set-up and accomplishment for MALDI Imaging analyses.

## Data analysis including database searching

General data analysis in SCiLS Lab, file export options, basics of MetaboScape, data transfer between SCiLS Lab and MetaboScape.

### **Applications**

Workflow for lipid or metabolite (if preferred peptide) and MALDI Imaging experiments on tissue.

## S4AA02 C4EL15

# solariX and scimaX series MRMS Metabolomics Application Course

## **Duration** 2 Days

#### Links

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#### Intention

This training course is intended for novice Bruker solariX series users without significant prior experience in metabolomics experiments. The course covers all specific aspects of data acquisition and data processing for metabolomics applications as well as application relevant HPLC aspects for metabolomics and small molecule applications such as lipids but does not substitute an explicit HPLC training.

#### **Prerequisite**

A MRMS Essential Operator Training Course should be passed before attending a metabolomics training course.

#### Location

Please check with your local Bruker Office where the training courses are offered.

Please note: This training does not replace a dedicated HPLC training!

## **Course Topics**

#### Introduction

Data acquisition of metabolomic samples including data processing using the scimaX MRMS instrument.

#### **ESI and MALDI**

ESI (Electrospray ionization) as well as MALDI measurements of different samples using positive and negative ion modes.

#### **Calibration and tuning**

Mass calibration, tuning of ion source and ion transfer parameters for these kind of samples in positive and negative ion mode.

#### **MS** operation

Mass resolution, speed, scan range, method handling, CASI, quadrupole isolation and fragmentation options.

#### Method handling and data acquisition

Method handling in ftmsControl, HyStar and DataAnalysis. Direct infusion measurements of standard metabolomic samples (polar compounds and lipids). Flow injection analysis (FIA) and LC-MS when required.

#### Data analysis

General data processing in DataAnalysis, processing of single spectra generated by MALDI, ESI or FIA experiments, SmartFormula calculation, MetaboScape workflow of FIA and LC-MS data.

#### **Applications**

Analysis of metabolomic samples such as tea and coffee extracts in MetaboScape. Specific requirements of the customer with respect to the focus of this course will be discussed.

## S4AA02 C4EP15

## solariX and scimaX series MRMS Petroleomics Application Course

## **Duration** 2 Days

#### Links

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#### Intention

This training course is intended for novice Bruker solariX series users without significant prior experience in petroleomics experiments. The course covers all important aspects of data acquisition and data processing for petroleomics applications using different ionization techniques such as APPI, APCI and LDI.

#### **Prerequisite**

A MRMS Essential Operator Training Course should be passed before attending a petroleomics training course.

#### Location

Please check with your local Bruker Office where the training courses are offered.

## **Course Topics**

#### Introduction

Data acquisition of petroleomics samples including data processing using the scimaX MRMS instrument.

## Atmospheric pressure ionization (API) and LDI

API techniques (ESI/APCI/APPI) as well as laser desorption ionization (LDI), ionization efficiency, direct infusion (DI) and flow injection analysis (FIA) (optional).

#### **Calibration and tuning**

Mass calibration, tuning of ion source and ion transfer parameters for these kind of samples in positive and negative ion modes.

#### **MS** operation

Mass resolution, detection range, method handling, CASI, quadrupole isolation and CID fragmentation.

#### Method handling and data acquisition

Method handling in ftmsControl, HyStar (optional for FIA) and DataAnalysis. Acquisition of petroleomics data via APPI and LDI.

#### **Data analysis**

General data processing in DataAnalysis, processing of petroleomics spectra with 3rd party software such as Composer\* or PetroOrg\*\* software. Generation of specific plots such as DBE vs. C, Van Krevelen plots etc. Export of processing results as Excel sheets.

#### **Applications**

Analysis of petroleomics samples using LDI as well as APCI and APPI via direct infusion experiments. Specific requirements of the customer with respect to the focus of this course will be discussed.

<sup>\*</sup> Composer is a product of Sierra Analytics, Modesto, CA 95356 USA

<sup>\*\*</sup> PetroOrg is a product of National High Magnetic Field Laboratory, Tallahassee, Florida

## S4AA02 C4EL15

# solariX and scimaX series MRMS Biomolecules Application Course

## **Duration** 2 Days

#### Links

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#### Intention

This training course is intended for novice Bruker solariX series users without significant prior experience in biomolecule experiments. The course covers all important aspects of data acquisition and data processing for biomolecule applications using MALDI and ESI, as well as different fragmentation techniques such as CID, ETD and ECD.

#### **Prerequisite**

A MRMS Essential Operator Training Course should be passed before attending a metabolomics training course.

## **Course Topics**

#### Introduction

Data acquisition of biomolecule samples including data processing using the scimaX MRMS instrument.

#### **ESI and MALDI**

ESI (Electrospray ionization) and MALDI (Matrix-assisted laser/desorption ionization) measurements of different biomolecule samples. Fragmentation techniques: Collision Induced Dissociation (CID), Electron Transfer Dissociation (ETD) and Electron Capture Dissociation (ECD) of peptides and proteins.

#### **Calibration and tuning**

Mass calibration, tuning of ion source and ion transfer parameters for these kind of samples in positive and negative ion mode.

#### **MS** operation

Mass resolution, detection range, method handling, Continous Accumulation of Selected lons (CASI), quadrupole isolation, CID, ETD and ECD fragmentation.

#### Method handling and data acquisition

Method handling in ftmsControl, HyStar (optional for LCMS) and DataAnalysis. Acquire protein digest spectra and generate MS/MS fragmentation data.

#### **Data analysis**

General data processing in DataAnalysis, processing of peptide mass fingerprint (PMF) and fragmentation data (CID, ETD and ECD) in BioTools. Database search via MASCOT.

#### **Applications**

Analysis of biomolecule samples using MALDI and ESI. Specific requirements with respect to the focus of the course will be discussed.

## **ESI Ion Trap Operator**

Training courses cover the range from instrument control to application driven solution

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#### **C2EL13**

# **Ion Trap Essential Operator Training Course**

## **Duration** 2.5 Days

## Low Molecular Weight Applications

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#### Intention

This training course is intended for novice Bruker ion trap users without significant prior experience in data acquisition, data analysis and instrument maintenance. The course covers all important aspects of ion trap operation and data processing as well as application relevant HPLC aspects but does not substitute an explicit HPLC training.

#### **Prerequisite**

Due to the familiarization during system installation, attendees should have a basic knowledge of the ion trap mass spectrometer with several weeks of practical experience with the instrument and software.

Please note: This training does not replace a dedicated HPLC training!

## **Course Topics**

#### Introduction

Theory of the ion trap mass spectrometry and atmospheric pressure ionization (API) techniques.

Atmospheric pressure ionization (API), Electrospray Ionization (ESI) and alternative API techniques (IonBooster/APCI/APPI), ionization efficiency, direct infusion and HPLC-ESI-MS coupling.

#### **Calibration and tuning**

Calibration (e.g. detector, scan modes), tuning of the ion transfer with special focus on small molecules, positive/negative switching.

#### Ion trap and MS(n) operation

Scan modes, resolution and speed, scan range, Ion Charge Control (ICC), MS(n) capabilities of the ion trap, isolation and fragmentation options, Manual MS(n), MRM and data dependent MS(n) with intelligent precursor ion selection.

#### Method handling and data acquisition

Method handling in trapControl, HyStar and DataAnalysis. Set-up and accomplishment of HPLC MS<sup>n</sup> analyses.

#### **Data analysis**

General data processing in DataAnalysis, chromatogram trace definitions and MS(n) spectra extraction, FindCompounds algorithm, basic introduction to library search applications, QuantAnalysis™ software.

#### **Maintenance**

Good working conditions (solvents, containers, nitrogen etc.), cleaning of the ion source.

#### **Applications**

Small molecule analysis using LC-MS(n). Specific requirements of the customer with respect to the focus of this course will be discussed.

#### **C2ET12**

## **Toxtyper® Essential Operator Training Course**

## **Duration** 3 Days

## Toxtyper Routine Workflows

#### Links

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#### Intention

This training course is intended for novice users of the Bruker Toxtyper. It enables participants to perform the standard Toxtyper screening workflow. The course covers all important aspects of Toxtyper sample analyses, routine maintenance, instrument performance verification and Toxtyper QC measurements.

Another component of the training is the expansion of Toxtyper libraries with new drug compounds.

#### **Prerequisite**

Attendees should have a basic knowledge of LCMS coupling and the analysis of toxicological or forensic samples.

## Course Topics

#### Introduction

Introduction to HPLC and ion trap hardware as well as general features of the Toxtyper software.

#### **Toxtyper workflow**

Execution of the Toxtyper workflow according to the Toxtyper user tutorial. This includes LC-MS system setup, quality control samples, result interpretation based on real life samples and standby conditions.

## Routine Toxtyper ion trap performance tests

Weekly recommended maintenance tests of the system are trained: ESI source maintenance, detector check, and Toxtyper routine performance tests.

#### **Toxtyper ion trap calibrations**

After a brief introduction to the trapControl software calibrations of detector, scan calibration and isolation/fragmentation are performed.

#### **Troubleshooting**

Information on error handling is provided.

#### Additional topics on request

As add-ons more information on ESI and ion trap mass spectrometry can be given. Besides that, administrator options are discussed.

#### **C2EP13**

# **Ion Trap Essential Operator Training Course**

## **Duration** 3 Days

#### **Proteomics**

#### Links

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#### Intention

This training course is intended for novice Bruker ion trap users without significant prior experience in data acquisition, data analysis and instrument maintenance. The course covers all important aspects of ion trap operation and data processing as well as application relevant HPLC aspects but does not substitute an explicit HPLC training.

#### **Prerequisite**

Due to the familiarization during system installation, attendees should have a basic knowledge of the ion trap mass spectrometer with several weeks of practical experience with the instrument and software.

Please note: This training does not replace a dedicated HPLC training!

## **Course Topics**

#### Introduction

Theory of the ion trap mass spectrometry and electrospray ionization.

#### **Atmospheric pressure ionization (API)**

Electrospray Ionization (ESI) and nano ESI operation, ionization efficiency, direct infusion and HPLC-ESI-MS coupling.

#### **Calibration and tuning**

Calibration (e.g. detector, scan modes), tuning of the ion transfer with special focus on proteomics samples.

#### Ion trap and MS(n) operation

Scan modes, resolution and speed, scan range, Ion Charge Control (ICC), MS(n) capabilities of the ion trap, isolation and fragmentation options, data dependent MS(n) with intelligent precursor ion selection.

#### Method handling and data acquisition

Method handling in trapControl, HyStar and DataAnalysis. Set-up and accomplishment of HPLC MS(n) analyses.

#### **Data analysis**

General data processing in DataAnalysis, file export options, basics of BioTools/Protein-Scape software, protein identification via database search, automation.

#### **Maintenance**

Good working conditions (solvents, containers, nitrogen etc.), cleaning of the ion source.

#### **Applications**

Workflow for protein identification by data dependent LC-MS(n) analysis of tryptic digests. Specific requirements of the customer with respect to the focus of this course will be discussed.

#### **C2AA31**

# **Ion Trap Advanced Operator Training Course**

#### **Duration** 1 Day

Peptide Analysis using Electron Transfer Dissociation (ETD)

#### Links

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#### Intention

For users familiar with Bruker ion trap ETD systems who want to start with ETD analyses.

#### **Prerequisite**

Participants should have attended an Ion Trap Essential Operator Training Course "Proteomics Applications".

## **Course Topics**

## Introduction to Electron Transfer Dissociation (ETD) and Proton Transfer Reaction (PTR)

Principles of ETD, ETD fragmentation mechanism, differences between ETD and CID, nCl source configuration and function.

#### **ETD** and **PTR** operation

Overview on ETD software features, tuning of nCl source parameters for ETD and PTR operation.

#### **ETD** acquisition modes

Manual and data dependent ETD, alternating CID-ETD analysis, neutral loss triggered ETD (PTMScan™), SmartDecomposition for bottom-up analysis of post-translational modifications (PTMs).

#### **Data analysis**

Data processing in DataAnalysis, file export options.

#### **BioTools (BioPharma Compass®)**

Handling of ETD data in either BioTools / ProteinScape® or BioPharma Compass.

#### **Applications**

Analysis of phosphopeptides by data dependent LC-MS(n) using CID and ETD. Specific requirements with respect to the focus of this course will be discussed.

## **SPR Operator**

Training courses cover the range from instrument control to application driven solution

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#### **D1EX01**

# **SPR Essential Operator Training Course**

## **Duration** 2 Days

#### SPR Pro Instruments

#### Links

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#### Intention

This training course focuses on the basics of practical SPR operation with focus on the determination of kinetic constants. The course covers the essentials of sample preparation, data acquisition/processing and instrument maintenance. Thus, the course will enable novice users getting started with SPR analyses.

The course will be held onsite of the customer using the installed instrumentation. This ensures that all applications trained during the course will for sure be applicable on the local installation.

The number of customers trained during this training is defined by the customer's requirements. However, for practical and didactical reasons, groups should not get larger than 5 trainees.

#### **Prerequisite**

Basic general knowledge in SPR is highly recommended and lab experience required. Attendees of the training course are encouraged to take part in the user familiarization that is done at a customer site upon installation of the SPR instrument.

#### Required infrastructure onsite

Access to the system, max. 5 people per training.

Customer provides general lab equipment and access to D2O.

## Course Topics

## The training content in its fullest extend would be as following:

#### **Basics in SPR**

Basic training on the theory of SPR and the different applications with SPR. Individual questions and specific requirements with respect to the focus of this course will be discussed.

#### Instrument overview

Familiarization with the SPR systems and its features for the different applications as well as the handling of the instrument.

General maintenance of the SPR instrument, including methods of cleaning and cleaning routines.

#### **Data acquisition software training**

Introduction into the handling of the data acquisition software (SPR Control Software) and joint generation of selected basic methods.

#### **Practical training**

Practical training on system with two kinetic test assays (incl. method programming and sample handling).

The experiments include coverage of method creations incl. racks, sensor docking and precondition, pH-scouting, protein immobilization and kinetic experiment.

#### **Data analysis**

General data processing and evaluation using Sierra SPR Analyzer Software, introduction to SPR analysis software and practical training on data analysis from the obtained assay data. Discussion of application specific software questions.

#### **D3AX01**

# **SPR Individual Operator Onsite Training Course**

#### **Duration**

Up to 3 Days

#### Links

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## Available from O2 / 2023

#### Intention

This trainings course focuses on your individual needs and will cover the topics that you request upfront.

From a simple operator refresh training to a deep dive into Analyzer and Control Software over a focus on assay optimization to method development for your specific application, the course will be individually fitted.

#### **Prerequisite**

Attendees need to have completed the basic SPR Essential Training Course and participated in the user familiarization done at a customer site upon installation of the SPR instrument.

Not more than 5 attendees for practical work!

#### Required infrastructure

Sample material for the application of interest has to be provided by the customer.

## **Course Topics**

## The training content will be fitted to your individual needs and can feature:

#### **Assay discussion (virtual)**

We discuss your application 4-6 weeks before the actual training in a virtual meeting. This meeting serves the purposes to define the scope of the training and identify necessary reagents for the assay. These should then be organized by the customer until the onsite training takes place.

#### Theoretical introduction to application

The theoretical background for the specific training application is discussed in-depth in a lecture (1-2 hours) in a virtual meeting. A recording is then provided to the customer.

## Assay development and optimization support

Our specialists support you with initial assay development or assay optimization and show you methods to make assay development for SPR Pro instruments easier and more comfortable.

#### **Specific application training**

The training focuses on a specific application discussed upfront. This training is done with customer samples and should enable the user to eventually perform as well as improve the assay of interest independently. An extensive assay optimization may be included, but is not necessary.

Specific application trainings are offered for these applications:

- Concentration Analysis
- Kinetic Assay for Protein-protein Interactions
- Kinetic Assay for Small Molecule-protein Interactions
- Thermodynamics
- Screening
- Conditional Binding
- Epitope Binning

## **Software courses**

Training courses cover different software in depth for comprehensive knowledge and maximized efficiency

**Online Operator/Inhouse Training Courses** 

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## C9AA21 Software courses

## **Duration** 2 x 0.5 Days - online

## Statistical analysis of MALDI imaging data using SCiLS™ Lab software

#### Links

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#### Intention

This training course provides a comprehensive introduction to the statistical analysis of imaging mass spectrometry data using the SCiLS Lab software.

#### **Prerequisite**

Attendees should be well familiar with the principle of imaging mass spectrometry. Users of Bruker MALDI mass spectrometers, ideally, should have completed an Essential Operator Training course MALDI Imaging.

## Course Topics

- Data import options in SCiLS™ Lab
- Adjusting general settings and file properties
- Fully automated pipeline for unsupervised, multivariate analysis of imaging data (Segmentation)
- Application of further statistical methods of univariate and multivariate, unsupervised and supervised statistical data analysis (ROC, component analysis, colocalization analysis)
- Semi-supervised classification of spectra cohorts based on statistical models
- SCiLS™ Lab Report Table

## C1AS11 Software courses

## **Duration** 0.5 Days - online

## Polymer analysis using PolyTools

#### Links

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#### Intention

This training course addresses users of Bruker MALDI-TOF/TOF instruments working in the field of synthetic polymer analysis. The course focuses on Bruker's PolyTools software and how to use it for the in-depth analysis of MS and MS/MS data obtained from polymer samples.

#### **Prerequisite**

Participants should have a basic knowledge of mass spectrometry-based workflows applied to polymer analysis.

## Course Topics

#### Introduction and data import

Introduction PolyTools top-level functionalities and introduction of the main workflows which are supported.

#### **Feature table computation**

Definition of processing parameters to perform peak picking, retention time alignment, deconvolution, data recalibration, and recursive feature extraction.

#### **Feature finding**

Characterization of polymers based on their key features such as number-average molar mass Mn, mass-average molar mass Mw and dispersity. Analysis of end groups is discussed.

#### **Statistics**

Advantages of various Kendrick Mass Plots are explained: Standard KMD plot with the resolution enhanced option (KMD vs m/z), Kendrick Mass Defect vs Remainder of Nominal Kendrick Mass (RNKM), Remainders of Kendrick Mass (RKM) vs. m/z– Remainders of Kendrick Mass (RKM) vs. Remainder of Nominal Kendrick Mass (RNKM).

#### Data revision, filter, and export options

The influence of parameter settings for the graphical display as well as data exporting for further data analysis are demonstrated.

## C9AA21 Software courses

## **Duration** 2 x 0.5 Days - online

## MetaboScape®

#### Links

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#### Intention

For users familiar with Bruker ESI-QTOF systems, timsTOF systems (including imaging data aquired on timsTOF fleX) or MRMS systems who want to successfully use the MetaboScape software for statistical analysis and compound identification in Metabolomics applications.

#### **Prerequisite**

Attendees should have a basic knowledge of ESI-QTOF or MRMS mass spectrometry with several weeks of experience with the instrument and the software. Additionally, they should have attended an Essential Operator Training course "Low molecular weight applications", previously. Basic knowledge about statistics is of advantage.

## **Course Topics**

#### **Introduction and Data Import**

Introduction to the general software functionalities and main supported workflow. Steps to import Data-Dependent-Acquisition (DDA) experiments and definition of sample groups for statistics.

#### **Feature table computation**

Definition of processing parameters to perform peak picking, retention time alignment, deconvolution, data recalibration, and recursive feature extraction.

#### **Feature annotation**

Identification of compounds using different tools, such as matching with spectral libraries, target lists, SmartFormula and SmartFormula3D, Biotransformer, rule-based lipid annotation, CompoundCrawler, and in silico fragmentation using MetFrag.

#### **Statistics**

Use of statistical tests included in MetaboScape such as for univariate statistics (t-Test/Wilcoxon test, ANOVA/Kruskal-Wallis test), and multivariate statistics (Principal Component Analysis, Partial Least Square, hierarchical clustering).

#### Pathway mapping

Targeted search of identified compounds in pathways of interested using a built-in MetaboScape tool.

#### Data revision, filter, and export options

Introduction to the tools to differentially visualize data with graphs, as well as to filter features based on various rules using flags or direct exclusion before data exporting.

## C9AA61 Software courses

## **Duration** 2 x 0.5 Days - online

### **TASQ®**

#### Links

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#### Intention

This training course addresses users of Bruker mass spectrometry instruments working in the field of screening applications. The course focuses on Bruker's TASQ software and how to use it for organizing, and analyzing screening data.

#### **Prerequisite**

For users familiar with Bruker ESI-QTOF, ESI-timsTOF or ESI-TQ systems who want to use the TASQ® software for screening and quantitation applications.

## Course Topics

#### Introduction

Introduction to the TASQ workflows, prerequisites for data processing and most important functionalities.

#### **General workflow**

The general workflow of importing, processing, reviewing and quantitation of batches will be demonstrated.

#### **Creating processing methods**

The general method setting as well as analyte specific screening, scoring, integration, and quantitation settings are explained.

#### **Quantitation options**

The different quantitation options regular curve calibration with and without internal standards, single-point calibration, legacy calibration, surrogate quantitation, and standard addition will be demonstrated.

#### Reporting

Batch and analysis reports will be created.

## C9AA32 Software courses

## **Duration** 2 x 0.5 Days - online

## BioPharma Compass®

#### Links

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#### Intention

This training course addresses users of Bruker mass spectrometry instruments working in the field of proteomic analysis. The course focuses on Bruker's BioPharma Compass® software and how to use it for organizing, analyzing, and archiving of proteomics and glycomics data.

#### **Prerequisite**

Participants should have a basic knowledge of mass spectrometry-based workflows applied to proteomics / protein analysis.

### **Course Topics**

#### Introduction

Introduction to BioPharma Compass top-level functionalities and introduction of the main workflows which are supported.

#### **Administrative tasks**

Basic administrative tasks include user-, station-, workflow- and method management.

#### **Automation**

BioPharma Compass is a turnkey solution, meaning that the whole process of acquiring data, analysis of data, report generation and result storage is executed without the need of user intervention. In this section it is explained how this automation is implemented. The workflow and method concept is discussed, samples will be submitted, measured and analyzed. Finally, the available tools for inspecting results are customized and used.

#### Reprocessing and validation

The functionality for reprocessing of acquired data sets and validation of obtained results are discussed.

#### Workflows in detail

Details of the workflows Protein Screening, Top-Down ESI, Peptide Mapping, Peptide Mapping/PTM Comparison, Peptide Screening and Peptide Screening/Batch Comparison are presented.

#### **D2AX01**

# **SPR Software Online Training Course**

## **Duration** 0.5 Days

## SPR Pro Instruments, Analyzer and Control Software

#### Links

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#### Intention

This training course focuses on the introduction into the acquisition and analysis software of Bruker SPR (Control and Analyzer).

The course covers the essentials of how to create racks and methods with examples for the Control Software. Additionally, the essentials in how to perform a kinetic and quantification analysis including examples with the Analyzer Software are discussed.

Recommended for new users in your group.

#### **Prerequisite**

Internal resources to train the attendee on the practical handling with the Bruker SPR Pro instrument.

#### Required infrastructure remote

Access to both the Control and Analyzer Software can be beneficial, but is not needed.

## **Course Topics**

## The training content in its fullest extend would be as following:

#### Data acquisition software training

Introduction into the handling of the data acquisition software (SPR Control Software) and joint generation of selected basic methods.

#### Data analysis

General data processing and evaluation using Sierra SPR Analyzer Software, introduction to SPR analysis software and practical training on data analysis from assay data. Discussion of application specific software questions.

#### **C9AA61**

## **Onsite Training Courses**

#### **Duration**

Depends on the requirements different options available 2, 3, 4 or 5 Days

#### Links

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#### General

#### Intention

Nearly all courses are offered onsite at the customer facility as well. Each course can be tailored for the specific needs and requirements of the customers.

The course will be held onsite at the customer facility utilizing their installed instrumentation. This ensures that all the relevant applications the customer would like to cover during the course will be applicable on the local installation. The number of customers trained during this training is

defined by the customer's requirements. However, for practical and didactical reasons, groups should not be any larger than 5-6 trainees.

#### **Prerequisite**

Prerequisites depend on the actual training course content and should be discussed with the responsible application specialist from Bruker in advance of the training.

## Course Topics

As these training courses are specifically tailored according to our customer's requirements, a general course outline cannot be provided. This depends on instrument, topics to be covered as well as duration of the course and will be discussed with the Bruker application specialist in advance of the training course. Check for language availability.

Individual Onsite Training Courses	MALDI- TOF	Ion Trap	ΩТОF	timsTOF	timsTOF fleX	MRMS	GC-TQ	LC-TQ
2 Days	S1AA02	S2AA02	S3AA02	-	S8AA02	S4AA02	S6AA02	S7AA02
3 Days	S1AA03	S2AA03	S3AA03	S8AA03	S8AA03	S4AA03	S6AA03	S7AA03
4 Days	S1AA04	S2AA04	S3AA04	S8AA04	S8AA04	S4AA04	-	-
5 Days	S1AA05	-	S3AA05	S8AA05	S8AA05	S4AA05	-	-
	-							

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