



UNIVERSITY OF TARTU

# ValChrom open-access online validation software



Asko  
Laaniste

Developer of ValChrom  
11.12.2025



# ValChrom



## What:

Online software tool developed in University of Tartu, Chair of Analytical Chemistry.

## Purpose:

Proof of concept that chromatographic method validation can be largely automated.

## Uses:

1) MOOC „Validation of liquid chromatography mass spectrometry (LC-MS) methods“

Next iteration: **December 16, 2025 – February 27, 2026**. Free and open for registration.

2) Free to use for anyone who wants anywhere in the world.



## About me

### Asko Laaniste

- 2016. PhD in Analytical Chemistry
  - *Worked on initial version of ValChrom*
- 2016. – 2019. Worked in collaboration with University of Tartu and different private companies to solve chromatographic method development and validation challenges
  - *Further developed version of ValChrom*
- 2019. – 2023. BSc in *IT-systems development* in Tallinn University of Technology
  - *Thesis was on adding design of experiments (DoE) support to ValChrom*
- since 2021. Been working as fulltime software developer in University of Tartu and Nortal
  - *Developing ValChrom in University of Tartu*

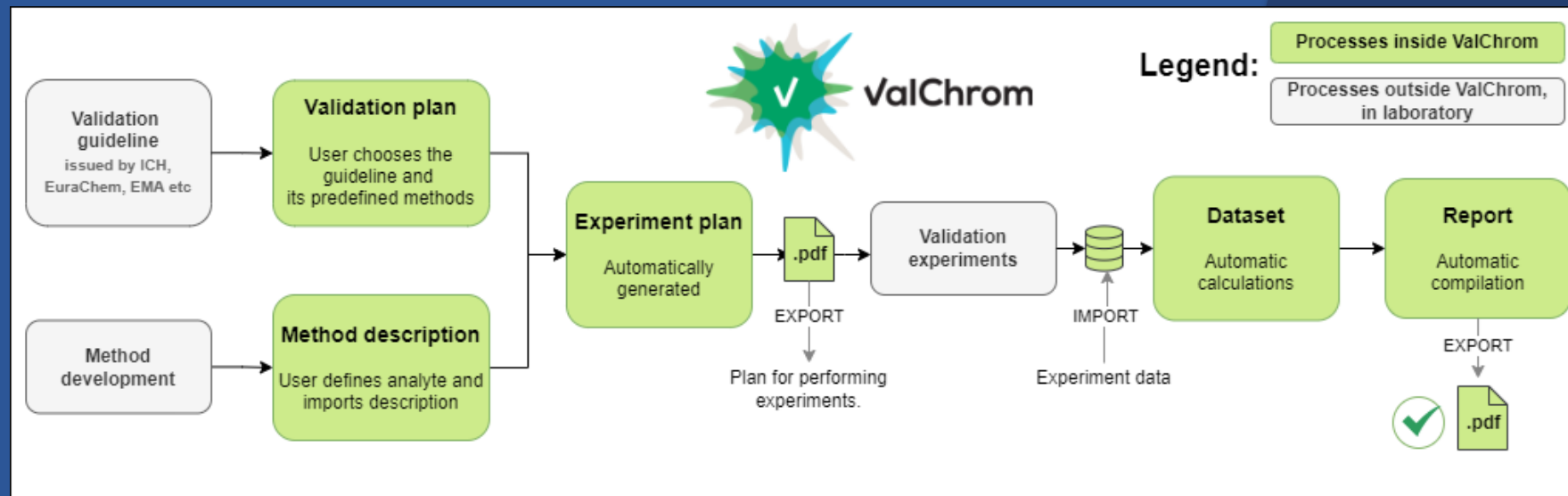
# Hands-on demo

Publicly available at <https://valchrom.ut.ee/>



Today we will:

- 1) Navigate to ValChrom
- 2) Use sample data
- 3) Breeze through the full flow

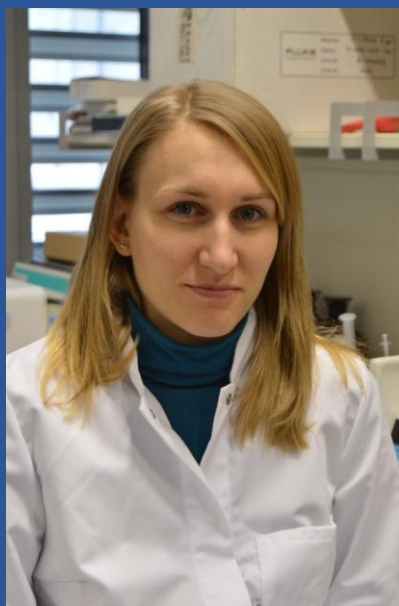
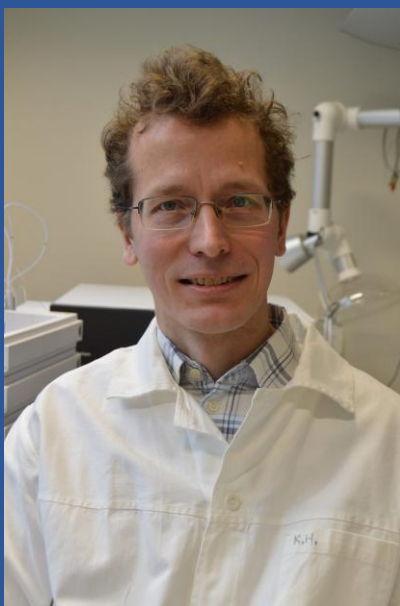




# ValChrom and MOOC team over the years



**ECAC** Estonian Center of  
Analytical Chemistry



# Thank you for your attention!

ValChrom: <https://valchrom.ut.ee>

MOOC: [https://sisu.ut.ee/lcms\\_method\\_validation](https://sisu.ut.ee/lcms_method_validation)



[Home](#) / [Sign Up](#)

## Sign Up

Create a new account

### My Details

*Passwords should be 8 or more characters and should contain at least 1 uppercase letter, 1 lowercase letter, a number and a symbol (!£\$%@?) e.g. Abcd1234&*

First name

Asko

Last name

Laaniste

Email

asko.laaniste@ut.ee

Password

.....

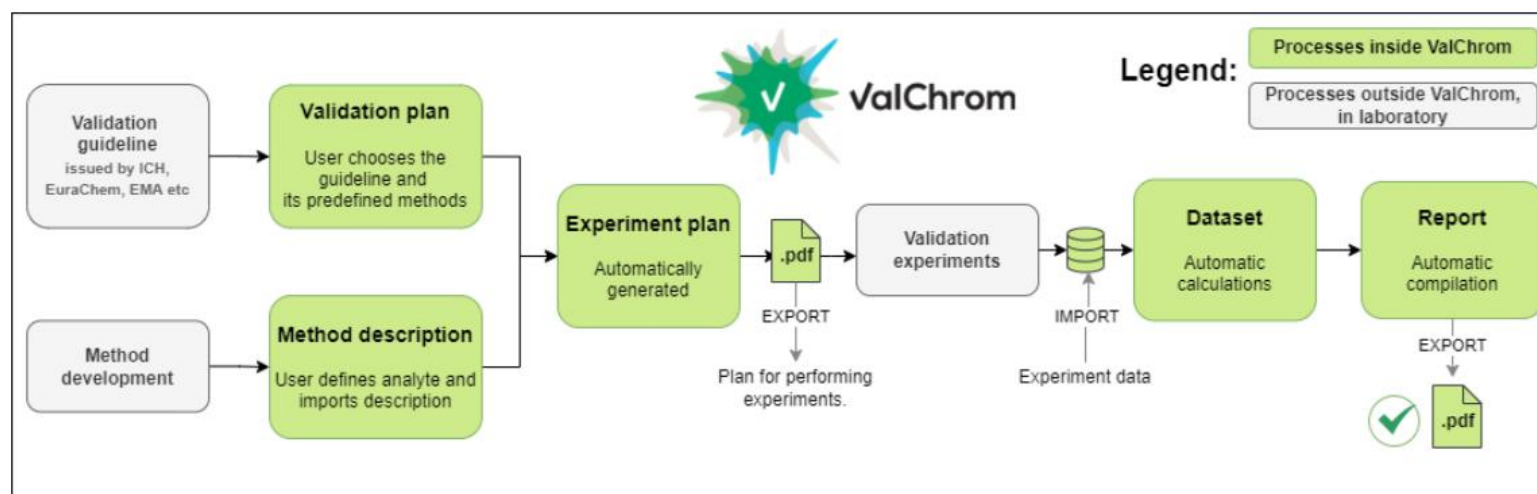
Confirm password

.....

Submit

Dashboard

# Dashboard





## Methods

### Active Methods

No Data To Show...

### Archived Methods

[Dashboard](#)[Analytical Methods](#)[Validation Plans](#)[Experimental Plans](#)[Experimental Datasets](#)[Reports](#)

## New Method

Method name\*

Workshop method

Concentration unit

ppb

Area unit

unitless

Retention time unit

min

Description

Demo method for workshop.

Add Analyte

Short Name

Official Name

Abbreviation

Target Concentration

Add

All Analytes

Short Name	Official Name	Abbreviation	Target Concentration	Action
ibuprofen	ibuprofen	IBU	1	Delete
ketoprofen	ketoprofen	KET	1	Delete

Method File (.zip):

Choose a file...

Method Description file (.pdf):

[Dashboard](#) / [Methods](#)

## Methods



### Active Methods

**Name****Status****Updated On** ▾**Action**[Workshop Method](#)

IN PROGRESS

09 December 2025

[Complete](#)

### Archived Methods



# Validation Plans

## Active Validation Plans

No Data To Show...

## Archived Validation Plans

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[Dashboard](#) / [Validation Plans](#) / New Validation Plan

## Create a new validation plan

Validation plan Name

Demo validation plan

Comment

Demo validation plan for workshop.

Select a guideline for your validation plan

☐ All assessment methods

☒ EMA BA

☐ Eurachem

☐ ICH

Continue

Cancel

Select a guideline for your validation plan

☐ All assessment methods

☒ EMA BA

☐ Eurachem

☐ ICH

## Validation Parameters

Selectivity ▼

LoD and LoQ ▼

Linear Range ▼

### Assessment method

☒ 3 series with 6 levels in parallel with blank and zero, matrix matched

#### Criteria:

☐ Minimum squared correlation coefficient (R2)

0.99

☒ Maximum back-calculated concentration error

0.15

☒ Maximum back-calculated concentration error for LoQ

0.2

☒ Back-calculated concentration - minimum number of levels

6

☒ Back-calculated concentration - minimum per cent of levels passing

0.75

☒ Back-calculated concentration - minimum per cent of parallels passing per level

0.5

☒ Lack-of-fit test

0

Precision ▼

## Validation Parameters

Selectivity ▼

LoD and LoQ ▼

Linear Range ▼

Precision ▼

### Assessment method

☒ Repeatability | 4 concentration levels with 5 parallels using LoQ, low, medium and high QC

#### Criteria:

☒ Maximum RSD 0.15

☒ Maximum RSD for LoQ 0.2

☒ Minimum number of parallels 5

☒ Minimum number of concentration levels 4

### Assessment method

☒ Intermediate precision | 3 series with 4 concentration levels on least 2 different days using LoQ, low, medium and high QC

#### Criteria:

☒ Minimum number of series 3

☒ Minimum number of concentration levels 4

☒ Maximum RSD 0.15

☒ Maximum RSD for LoQ 0.2

Accuracy ▼

Linear Range ▼

Precision ▼

Accuracy ▼

Assessment method

☒ Within-run: 4 concentration levels with 5 parallels using LOQ, low, medium and high QC.

Criteria:

☒ Within-run: Minimum number of parallels 5

☒ Within-run: Minimum number of concentration levels 4

☒ Minimum trueness 0.85

☒ Maximum trueness 1.15

☒ Minimum trueness for LoQ 0.8

☒ Maximum trueness for LoQ 1.2

Assessment method

☒ Between-run: 3 series with 4 concentration levels on least 2 different days using LoQ, low, medium and high QC

Criteria:

☒ Between-run: Minimum number of concentration levels 4

☒ Between-run: Minimum number of series 3

☒ Maximum trueness for LoQ 1.2

☒ Maximum trueness 1.15

☒ Minimum trueness 0.85

☒ Minimum trueness for LoQ 0.8






[Dashboard](#) / [Validation Plans](#)

# Validation Plans



## Active Validation Plans

Name	Status	Guideline	Updated On ↓	Action
<a href="#">Demo Validation Plan</a>	IN PROGRESS	EMA BA	09 December 2025	     <div>Complete</div>

## Archived Validation Plans

# Experimental Plans

## Active Experimental Plans

No Data To Show...

## Archived Experimental Plans

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[Dashboard](#) / [Experimental Plans](#)

# Experimental Plans

Active Experimental Plans

Archived Experimental Plans

## CREATE EXPERIMENTAL PLAN

**Plan name:****Analytical Method** ▾**Validation Plan** ▾**Create**

Cancel



Demo experimental plan

Analytical Method

Validation Plan | Demo validation plan

Experiment Plan

Title: Demo experimental plan

Total Days: 2 | Series: 3 | Experiments: 70

Current experiment plan is used to design and carry out analytical experiment for validation according to the choices user has made in validation plan. Experimental plan is devised for minimal number of chromatographic runs. The plan focuses on performing as many experiments as possible in one series. It is always possible to upload more than the minimum number of series (or levels or parallels, etc.).

+ Row

Rows

+ Column

Column

CSV

JSON

JSON

CSV

	Row #	Series		Day	Level	Sample Type		Parallel		Comment	
1		1		1	1	Calibration		1/2			
2		1		1	1	Calibration		2/2			
3		1		1	2	Calibration		1/2			
4		1		1	2	Calibration		2/2			
5		1		1	3	Calibration		1/2			
6		1		1	3	Calibration		2/2			

AI Assistant

Ask questions or request changes to your experiment plan

Start a conversation with the AI assistant

Ask questions or request changes to your experiment plan



## Demo experimental plan

### Analytical Method

### Validation Plan | Demo validation plan

### Experiment Plan

**Title:** Demo experimental plan

Current experiment plan is used to design and carry out analytical experiment for validation according to the minimum number of series (or levels or parallels, etc.).

+ Row    Rows   + Column    Column

▼	Row #	Series	▼	▼	Day	▼	Level	Sample Type	▼	Parallel	▼	Comment	▼
	1	1			1		1	Calibration		1/2			
	2	1			1		1	Calibration		2/2			
	3	1			1		2	Calibration		1/2			
	4	1			1		2	Calibration		2/2			
	5	1			1		3	Calibration		1/2			

#### Send message to AI service?

Your message and a snapshot of this experiment plan will be sent to a third-party AI service. Please do not include any sensitive or confidential information if you are not comfortable with this.

Cancel

I understand, continue

#### AI Assistant

Ask questions or request changes to your experiment plan



Start a conversation with the AI assistant  
Ask questions or request changes to your experiment plan

☒ Analysis Only   ☐ Allow Mutations

Ask about the plan or request changes...

Send

Press Enter to send, Shift+Enter for new line

## Demo experimental plan

## Analytical Method

## Validation Plan | Demo validation plan

## Experiment Plan

Title: Demo experimental plan

Total Days: 2 | Series: 3 | Experiments: 70

Current experiment plan is used to design and carry out analytical experiment for validation according to the choices user has made in validation plan. Experimental plan is devised for minimal number of chromatographic runs. The plan focuses on performing as many experiments as possible in one series. It is always possible to upload more than the minimum number of series (or levels or parallels, etc.).

+ Row

Rows

+ Column

Column

CSV

JSON

JSON

CSV

▼	Row #	Series	▼	▼	Day	▼	Level	Sample Type	▼	Parallel	▼	Comment
	1	1			1		1	Calibration		1/2		
	2	1			1		1	Calibration		2/2		
	3	1			1		2	Calibration		1/2		
	4	1			1		2	Calibration		2/2		
	5	1			1		3	Calibration		1/2		

## AI Assistant

Ask questions or request changes to your experiment plan

Explain what this plan determines and how to implement it in lab to validate LC-MS method.

10:30:00 PM

This experimental plan is designed for the validation of an LC-MS method, specifically focusing on assessing linearity, precision, and accuracy. It outlines the necessary runs to be performed across multiple series and days to meet the criteria defined in the associated validation guidelines (EMA BA in this case).

## Key Validation Aspects Determined by this Plan:

- 1. Linear Range (or "3 series with 6 levels in parallel with blank and zero, matrix matched"):** This part of the plan aims to establish the concentration range over which the method provides results that are directly proportional to the analyte concentration. It involves running calibration standards at 6 different concentration levels, in parallel, along with blank and zero samples. The data will be used to calculate the correlation coefficient (R2), assess back-calculated concentration errors, and ensure a sufficient number of levels and parallels meet predefined criteria.
- 2. Precision (Repeatability and Intermediate Precision):**
  - **Repeatability:** Assesses the variability of results when the same sample is analyzed multiple times under the same conditions (within a single run). The plan includes 4 concentration levels, each analyzed in 5 parallels.
  - **Intermediate Precision:** Evaluates variability under different within-laboratory conditions (e.g., different days, analysts, equipment). This plan schedules 3 series, each with 4 concentration levels, to be run on at least 2 different days.

☒ Analysis Only ☐ Allow Mutations

Ask about the plan or request changes...

Send

Press Enter to send, Shift+Enter for new line

Pending Changes

1 proposal

Total Changes: 72 Updates: 70

Added Updated Removed

Proposal 625fb4de  
Added 'Ibuprofen (IBU), ppb' and 'Ketoprofen (KET), ppb' columns with specified concentrations.

72 changes • Cols: 2 • Rows: 70 • Dec 9, 10:31 PM

+ Row

Rows

+ Column

Column

CSV

JSON

JSON

CSV

Actions	Row #	Series	Day	Level	Sample Type	Parallel	Comment	Ibuprofen (IBU), ppb	Ketoprofen (KET), ppb
<div>✓✗</div>	1	1	1	1	Calibration	1/2		2.4	0.01
<div>✓✗</div>	2	1	1	1	Calibration	2/2		2.4	0.01
<div>✓✗</div>	3	1	1	2	Calibration	1/2		29.7	0.155
<div>✓✗</div>	4	1	1	2	Calibration	2/2		29.7	0.155
<div>✓✗</div>	5	1	1	3	Calibration	1/2		57	0.305
<div>✓✗</div>	6	1	1	3	Calibration	2/2		57	0.305
<div>✓✗</div>	7	1	1	4	Calibration	1/2		84.3	0.455
<div>✓✗</div>	8	1	1	4	Calibration	2/2		84.3	0.455
<div>✓✗</div>	9	1	1	5	Calibration	1/2		111.6	0.5
<div>✓✗</div>	10	1	1	5	Calibration	2/2		111.6	0.5
<div>✓✗</div>	11	1	1	6	Calibration	1/2		120	0.5
<div>✓✗</div>	12	1	1	6	Calibration	2/2		120	0.5
<div>✓✗</div>	13	1	1	7	Blank	1/1			

AI Assistant

Ask questions or request changes to your experiment plan

Add a new column called 'Ibuprofen (IBU), ppb' and fill its cells (not the level column but this new column only!) with concentrations like this: Ibuprofen (IBU) 4 sample concentration levels (ppb): 2.6, 7.8, 39, 78. Ibuprofen (IBU) calibration range (ppb) with the calibration points evenly distributed between this range within a series: 2.4 - 120 ppb AND Add another new column called 'Ketoprofen (KET), ppb' and fill its cells (not the level column but this new column only!) with concentrations like this: Ketoprofen (KET) sample concentration levels (ppb): 0.011, 0.0097, 0.049, 0.097. Ketoprofen (KET) calibration range (ppb) with the calibration points evenly distributed between this range within a series: 0.01 - 0.5 ppb.

10:31:29 PM

Added 'Ibuprofen (IBU), ppb' and 'Ketoprofen (KET), ppb' columns with specified concentrations.

10:31:46 PM

Proposed Changes

Added 'Ibuprofen (IBU), ppb' and 'Ketoprofen (KET), ppb' columns with specified concentrations.

- 2 column change(s)
- 70 workload change(s)

Accept Changes Reject

Analysis Only Allow Mutations

Ask about the plan or request changes...

Send






Press Enter to send, Shift+Enter for new line

[Dashboard](#) / [Experimental Plans](#)

## Experimental Plans



### Active Experimental Plans

Name	Status	Method	Template	Updated On ↓	Action
<a href="#">Demo Experimental Plan</a>	IN PROGRESS	Workshop Method	Demo Validation Plan	09 December 2025	<div><div></div><div></div><div></div><div></div><div></div></div> <div>Complete</div>

### Archived Experimental Plans





[Dashboard](#) / [Experimental Datasets](#)

## Experimental Datasets ?

### Active Experimental Datasets

No Data To Show...

### Archived ExperimentalDatasets

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[Dashboard](#) / [Experimental Datasets](#) / New Experimental Dataset

## New Experimental Dataset

Dataset name

Select an Experimental Plan

Demo experimental plan ▾

[View Analytical Method](#)[View Validation plan](#)

Next

Cancel

[Dashboard](#) / [Experimental Datasets](#) / [View Experimental Dataset](#)

## Experimental Dataset Details

<b>Name:</b>	Demo dataset
<b>Status:</b>	IN PROGRESS
<b>Experimental Plan:</b>	Demo experimental plan
<b>Created on:</b>	09 December 2025

[Bulk Upload](#)

### Validation Parameters

Linear Range ▾

#### Method of Assessment

3 series with 6 levels in parallel with blank and zero, matrix matched

[Upload data](#)

Precision ▾

#### Method of Assessment


[Dashboard](#) / [Experimental Datasets](#) / [View Experimental Dataset](#) / [View Input](#)

## Dataset upload


### Linear Range

3 series with 6 levels in parallel with blank and zero, matrix matched

Paste data:

 Click on the box, then Ctrl+V or "Paste"

Upload file (example template  ):

 Click to upload

/  Drag and drop here

Check data to proceed

Back

☐ Force linear regression to zero when intercept is small ( $< 2 \times$  intercept SD)

## Dataset preview (download as CSV )

line nr.	name	tr	area	expected concentration	level	series	marker	analyte	parallel
1	200x	21.869	13079	120.9649	1	2023-25-05	Calibration	IBU	1
2	200x	21.878	13217	120.9649	1	2023-25-05	Calibration	IBU	2
3	280x	21.846	9297	86.3677	2	2023-25-05	Calibration	IBU	1
4	280x	21.854	9176	86.3677	2	2023-25-05	Calibration	IBU	2
5	320x	21.869	8235	75.4089	3	2023-25-05	Calibration	IBU	1
6	320x	21.844	7954	75.4089	3	2023-25-05	Calibration	IBU	2
7	400x	21.844	6243	60.4825	4	2023-25-05	Calibration	IBU	1
8	400x	21.878	6489	60.4825	4	2023-25-05	Calibration	IBU	2

[Dashboard](#) / [Experimental Datasets](#) / [View Experimental Dataset](#) / Overview

## Overview

**Dataset name:** Demo dataset**Dataset status:** IN PROGRESS

Select an analyte to view its results

IBUPROFEN IBU ▾

Accuracy ▾

Linear Range ▾

Precision ▾

Select an analyte to view its results

IBUPROFEN IBU



Accuracy ▾

Within-run: 4 concentration levels with 5 parallels using LOQ, low, medium and high QC

Criteria	Limit	Found	Decision
Maximum trueness for LoQ	120.0%	122.0%	✗
Minimum trueness for LoQ	80.0%	101.0%	✓
Maximum trueness	115.0%	90.6%	✓
Minimum trueness	85.0%	69.4%	✗
Within-run: Minimum number of concentration levels	4	4	✓
Within-run: Minimum number of parallels	5	5	✓

Level	Trueness	SD (Data for trueness)	Pooled RSD (Data for trueness)
1	113%	7.68%	6.82%
2	86.8%	3.49%	4.02%
3	79.6%	7.29%	9.16%
4	76.2%	5.68%	7.46%

Series 2023-25-05

Criteria	Limit	Found	Decision
Maximum trueness for LoQ	120.0%	122.0%	✗
Minimum trueness for LoQ	80.0%	101.0%	✓
Maximum trueness	115.0%	90.6%	✓
Minimum trueness	85.0%	69.4%	✗
Within-run: Minimum number of concentration levels	4	4	✓
Within-run: Minimum number of parallels	5	5	✓

Select an analyte to view its results

IBUPROFEN IBU



Input data

Calibration data

Name	Level	Expected conc. (ppb)	tR (min)	Area (unitless)	Residual (unitless)	Back calculated concentration (ppb)	Back calculated concentration error
200x	1	121	23.4	2664	-55.1	119	-2.00%
200x	1	121	23.4	2772	52.9	123	1.92%
280x	2	86.4	23.4	1900	-31	85	-1.57%
280x	2	86.4	23.4	1955	24	87.4	1.22%
320x	3	75.4	23.4	1654	-27.3	74.2	-1.59%
320x	3	75.4	23.4	1724	42.7	77.3	2.48%
400x	4	60.5	23.5	1290	-51.3	58.2	-3.72%
400x	4	60.5	23.4	1386	44.7	62.4	3.24%
800x	5	30.2	23.4	630	-22.4	29.3	-3.26%
800x	5	30.2	23.4	677	24.6	31.3	3.56%
3320x	6	4.84	23.4	64	-9.8	4.41	-8.89%
3320x	6	4.84	23.4	65	-8.8	4.45	-7.98%
5000x	7	6.45	23.5	111	0.396	6.47	0.269%
5000x	7	6.45	23.4	131	20.4	7.35	13.9%
8000x	8	3.02	23.5	28	-4.29	2.83	-6.25%
8000x	8	3.02	23.4	36	3.71	3.18	5.40%
10000x	9	2.42	23.5	14	-4.69	2.21	-8.51%
10000x	9	2.42	23.4	20	1.31	2.48	2.38%

Series Overall

Slope (unitless / ppb)	Intercept (unitless)	F (calc.)	F (tabulated)	SD (slope, unitless / ppb)	SD (intercept, unitless)	R2	RSS
22.8	-36.4	0.0459	3.29	0.181	10.9	0.999	16321

Select an analysis to view its results

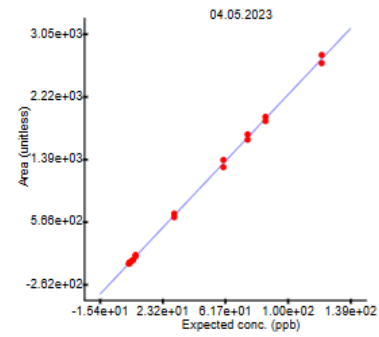
IBUPROFEN (BU)

10000x	9	2.42	23.5	14	-4.69	2.21	8.51%
10000x	9	2.42	23.4	20	1.31	2.48	2.38%

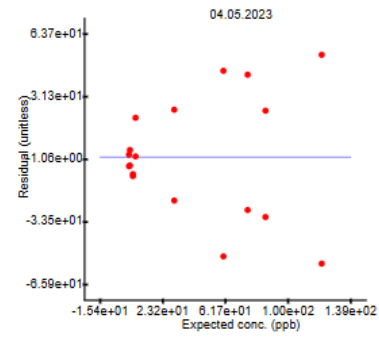
Series Overall

Slope (unitless / ppb)	Intercept (unitless)	F (calc.)	F (tabulated)	SD (slope, unitless / ppb)	SD (intercept, unitless)	R2	RSS
22.8	-96.4	0.0459	3.29	0.181	10.9	0.999	16321

Linear regression graph



Residuals graph





[Dashboard](#) / [Reports](#)

## Reports



Filter reports by dataset

All datasets ▾

No Data To Show...

- Dashboard
- Analytical Methods
- Validation Plans
- Experimental Plans
- Experimental Datasets
- Reports



[Dashboard](#) / [Reports](#)

# Reports

All datasets

## Select a dataset

Report name

Demo report

Dataset

Demo dataset ▾

Cancel

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Generate PDF

Generate .docx

Summary table

Mode Counts (editable)

Toolbox

Download Draft

Upload Draft

Images

Drop files onto the document or click below to insert at the selected line.

Add Image

Filters

Toggle what content is shown.

Analytes

Select All Clear

- ☐ ibuprofen  
☐ ketoprofen

Parameters

Select All Clear

- ☐ Linear Range  
☐ Precision

### Validation summary by analyte

Analyte	Criteria passed	Decision
ibuprofen	41/48	FAIL
ketoprofen	43/48	FAIL

Page BreakPage Break

### IBUPROFEN

#### Linear Range

#### 3 series with 6 levels in replicate with blank and zero, matrix matched

Measurements are made in three series using six replicated levels under matrix-matched conditions and including both blank and zero samples. This design supports assessment of selectivity, matrix effects and linearity with appropriate treatment of zero and blank responses.

#### Criteria

Name	Limit	Found	Decision
Lack-of-fit test	3.29	0.0459	✓
Back-calculated concentration - minimum per cent of parallels passing per level	50.0%	100.0%	✓
Back-calculated concentration - minimum per cent of levels passing	75.0%	100.0%	✓
Back-calculated concentration - minimum number of levels	6	9	✓
Maximum back-calculated concentration error for LoQ	20.0%	-8.51%	✓
Maximum back-calculated concentration error	15.0%	13.9%	✓

#### Calibration data for series '04.05.2023'



ValChrom

Report Builder

Filters are active. Adding, reordering, and draft upload/download

Generate PDF

Generating .docx

Generating document, please wait... ~38s remaining

Summary table

Mode Counts (editable) ▼

Toolbox

Download  
Draft

Upload  
Draft

Images

Validation summary by analyte

Analyte
ketoprofen

KETOPROFEN

Linear Range

3 series with 6 levels in replicate with blank and zero samples

Measurements are made in three series using six replicates per level. This design supports assessment of selectivity and response.

Criteria

*Validation summary by analyte*

Analyte	Criteria passed	Decision
ketoprofen	43/48	FAIL

**KETOPROFEN****Linear Range****3 series with 6 levels in replicate with blank and zero, matrix matched**

Measurements are made in three series using six replicated levels under matrix-matched conditions and including both blank and zero samples. This design supports assessment of selectivity, matrix effects and linearity with appropriate treatment of zero and blank responses.

*Criteria*

Name	Limit	Found	Decision
Lack-of-fit test	3.29	0.786	✓
Back-calculated concentration - minimum per cent of parallels passing per level	50.0%	100.0%	✓
Back-calculated concentration - minimum per cent of levels passing	75.0%	100.0%	✓
Back-calculated concentration - minimum number of levels	6	9	✓
Maximum back-calculated concentration error for LoQ	20.0%	14.2%	✓
Maximum back-calculated concentration error	15.0%	11.7%	✓

*Calibration data for series '04.05.2023'*

Name	Level	Expected conc. (ppb)	tR (min)	Area (unitless)	Residual (unitless)	Back calculated concentration (ppb)	Back calculated concentration error
200x	1	0.5038	17.076	11817	32.80292528	0.5024141395	-0.275%
200x	1	0.5038	17.059	11991	141.1970747	0.509765305	1.18%
280x	2	0.3597	17.076	8360	78.99687359	0.3563625339	-0.928%
280x	2	0.3597	17.059	8703	264.0031264	0.3708536247	3.10%
320x	3	0.3141	17.076	7186	173.6578316	0.3067632904	-2.34%
320x	3	0.3141	17.068	7338	21.65783155	0.3131849982	-0.291%
400x	4	0.2519	17.059	5719	168.4015067	0.24478536	-2.82%

# Welcome

ValChrom is free to use and only requirement is for users to sign up (the emails are used in order to send notifications if major changes are implemented).

Test user

email: testuser@testuser.ee

password: testuser

Demo materials: demo.zip

**To start with ValChrom: tutorial materials.**

**To start with Design of Experiments: [DoE service](#).**

ValChrom is under ongoing development. Any feedback on how to improve the software or any suggestions for additional functionality is greatly appreciated at valchrom@ut.ee or +372 737 6030.

Validation is used for testing how well different methods fit for purpose. Several international organizations have set different criteria for validation of chromatographic methods in their corresponding guidelines. We are developing a software named ValChrom that enables the user to follow a chosen guideline. This guidance has been achieved by directing the user through several choices that apply for different guidelines. The ValChrom software enables to calculate different validation parameters based on users' input data.

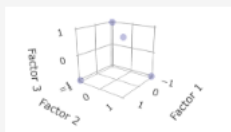
[Help me choose](#)**Design of Experiments**

Designs

Import

Results

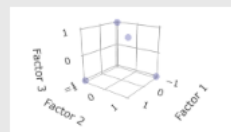
## Screening



### Plackett-Burman Designs

Plackett-Burman designs are efficient screening designs allowing the identification of significant factors with a minimal number of experimental runs. Particularly useful for preliminary experiments with the primary goal of understanding the effects of numerous factors, without requiring extensive resources and time.

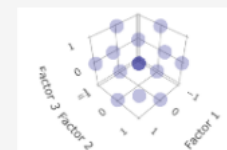
Info about this design at NIST/SEMATECH e-Handbook of Statistical Methods



### Fractional-Factorial Designs

Fractional Factorial Designs allow investigation of factors' effects with fewer experimental runs, while still providing valuable insights into influential factors. Particularly useful in screening experiments to identify key factors for further detailed study or optimisation.

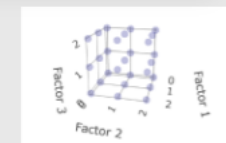
Info about this design at NIST/SEMATECH e-Handbook of Statistical Methods



### Box-Behnken Designs

Box-Behnken designs provide a balance between the number of experimental runs and the quality of the results, making them ideal for optimization studies.

Info about this design at NIST/SEMATECH e-Handbook of Statistical Methods



### Full Factorial Designs

Full Factorial designs consider all possible combinations of factors and levels. Can be resource-intensive, but they offer a complete understanding of the relationships between variables in an experimental setting.

Info about this design at NIST/SEMATECH e-Handbook of Statistical Methods



## Parameters (3)



Factor 1

-1 = NA

1 = NA

0 = NA

Factor 2

-1 = NA

1 = NA

0 = NA

Factor 3

0 = NA

-1 = NA

1 = NA

Factors: 3

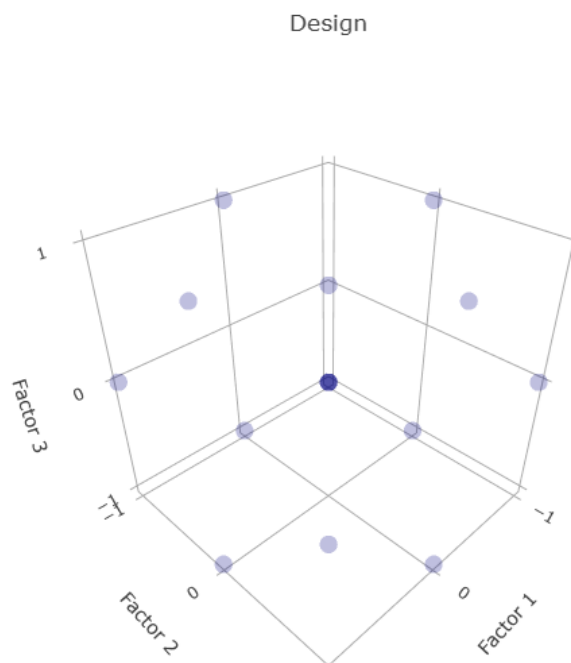


Center point measurements: 4



Export to CSV

#	Factor 1	Factor 2	Factor 3
1	-1	-1	0
2	1	-1	0
3	-1	1	0
4	1	1	0
5	-1	0	-1
6	1	0	-1
7	-1	0	1
8	1	0	1
9	0	-1	-1
10	0	1	-1
11	0	-1	1
12	0	1	1
13	0	0	0
14	0	0	0
15	0	0	0
16	0	0	0



<<<





## Factors (3)



Concentration

Time

Temp

## Responses (2)

Area\_thiacloprid

Area\_acetamiprid

Paste here

Calculate results and view



#	Factor: Concentration	Factor: Time	Factor: Temp	Response: Area_thiacloprid	Response: Area_acetamiprid
1	1	1	1	12	145
2	1	1	-1	2	221
3	1	-1	1	3	300
4	1	-1	-1	14	218
5	-1	1	1	29	234
6	-1	1	-1	22	159
7	-1	-1	1	14	400
8	-1	-1	-1	20	512
9	0	0	0	33	65
10	0	0	0	35	78
11	0	0	0	32	88

<<<





Summary

Graphs

### Summary of the predictive model for "Area\_thiacloprid"

F-test conclusion: The model is significant. (F-statistic: 73.17, p-value: 1.355e-2)

ANOVA test conclusion: There are factors with statistically significant effect on the response variable.

#### Significant factors:

- Concentration
- Concentration\*Time
- Time\*Temp
- Concentration<sup>2</sup>
- Time<sup>2</sup>
- Temp<sup>2</sup>

#### Insignificant factors:

- Concentration\*Temp
- Temp
- Concentration\*Time\*Temp
- Time
- Intercept

Raw data ▾

### Predictive model for "Area\_thiacloprid"

#### Significant factors

Area\_thiacloprid =  
(-6.75)\*Concentration  
+(-6.28)\*Time<sup>2</sup>  
+(-6.28)\*Concentration<sup>2</sup>  
+(-6.28)\*Temp<sup>2</sup>  
+(-2.50)\*Concentration\*Time  
+4.25\*Time\*Temp

#### All factors and interactions (adj. r<sup>2</sup>: 0.98, r<sup>2</sup>: 1.00)

Area\_thiacloprid = (-6.75)\*Concentration  
+(-6.28)\*Time<sup>2</sup>  
+(-6.28)\*Concentration<sup>2</sup>  
+(-6.28)\*Temp<sup>2</sup>  
+(-2.50)\*Concentration\*Time  
+(-0.25)\*Concentration\*Temp  
+0.00\*Temp  
+1.00\*Concentration\*Time\*Temp  
+1.75\*Time  
+4.25\*Time\*Temp  
+33.33\*Intercept



Summary Graphs

Factors

- ☒ Time
- ☐ Concentration
- ☐ Temp

Responses

- ☒ Area\_thiacloprid
- ☐ Area\_acetamiprid

Types

- ☒ Half-Normal plot
- ☒ Pareto plot
- ☒ Surface plot
- ☒ Contour plot

Graph options

Graph Size: 461

