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Changing Basis Sets: A Computational Chemist's Journey into Start-up World

Davor Šakić, PhD
Co-founder, CEO

May, 2026.

Computational Chemistry Day

Prerequisites

Journal of COMPUTATIONAL CHEMISTRY

Stochastic search for isomers on a quantum mechanical surface

Martin Saunders

First published: 15 January 2004 | https://doi.org/10.1002/jcc.10407 | VIEW METRICS

Acknowledgment

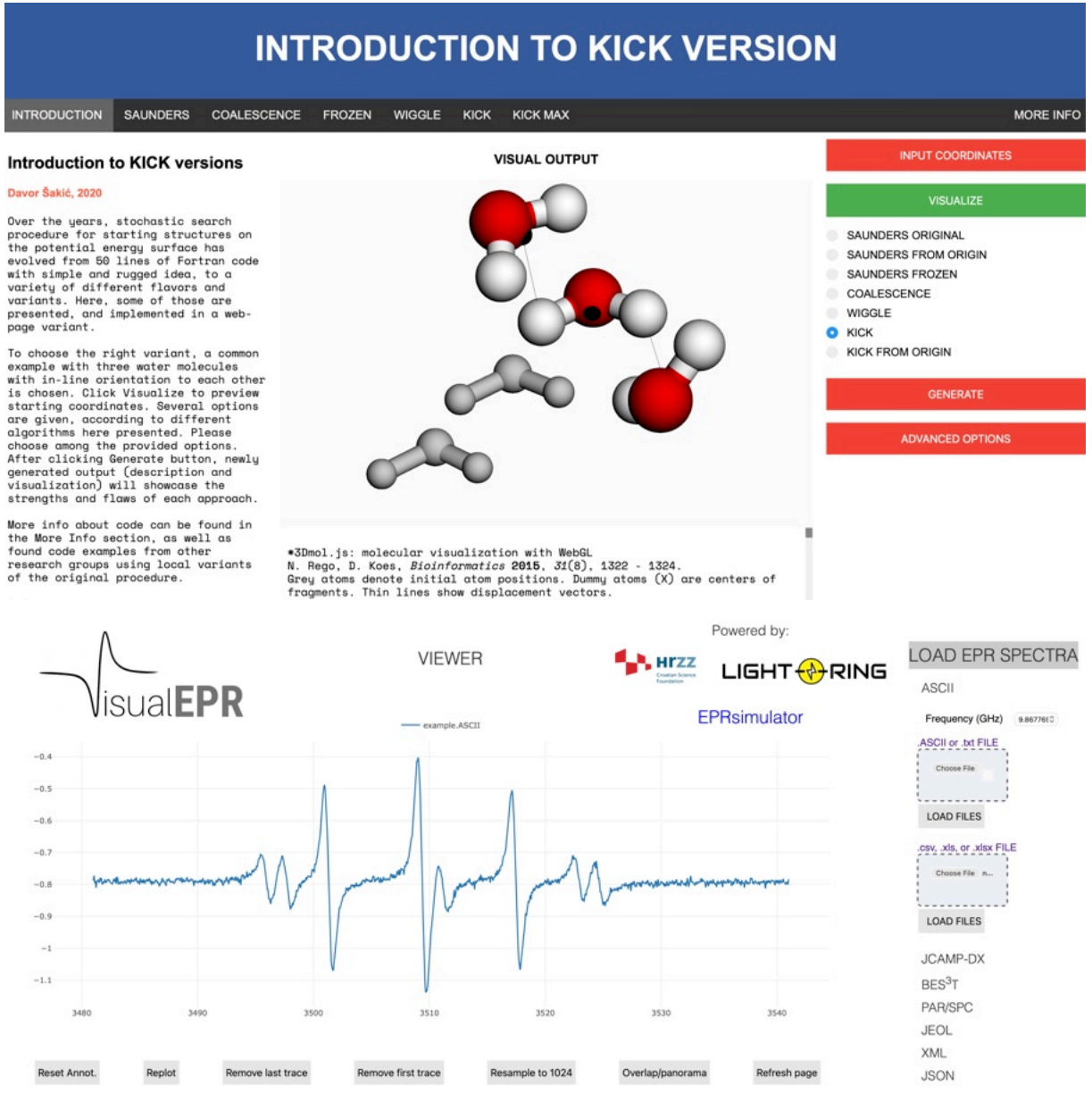
The author thanks Paul Schleyer for valuable comments on this article.

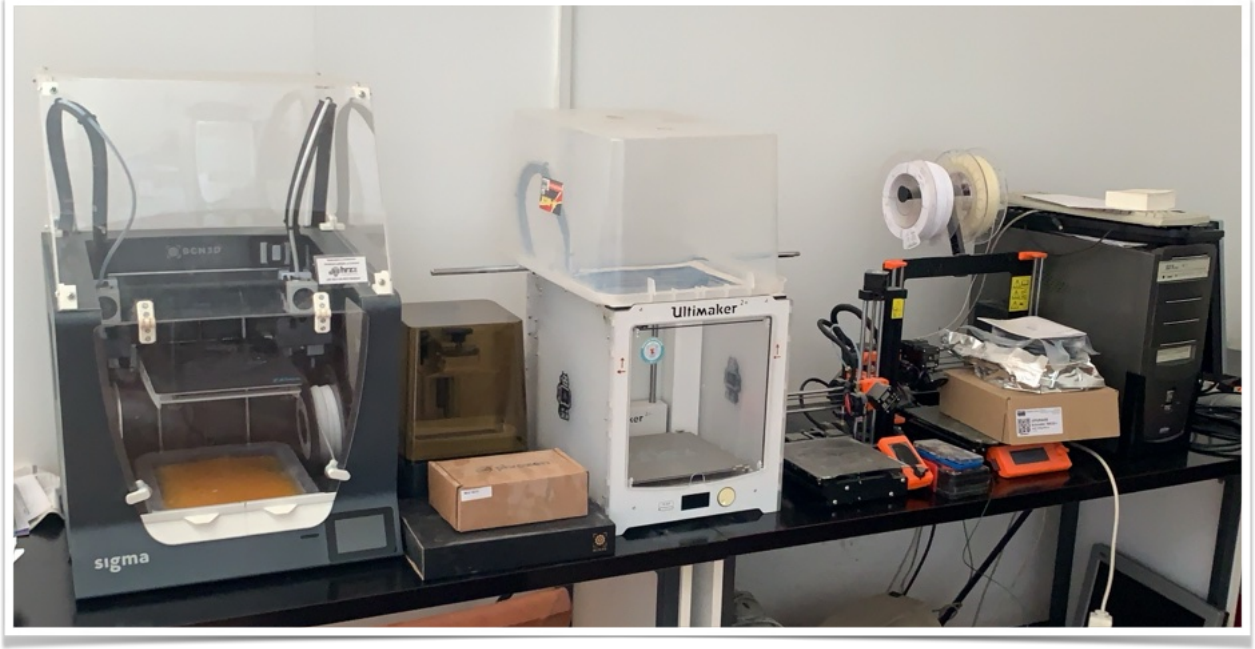
Appendix

```
      DIMENSION x(100), y(100), z(100), x1(100),
        y1(100), z1(100)
      integer*4 iseed
      character*80 a1, name
      character*12 fname
      character*1 e1 (100)
      open (21, file = 'kicksize.tx', status =
        'old')
      open (23, file = 'kicked.gjf', status =
        'unknown')
      read (21, 21) rad, name
21    format (f10.0, /a)
      fname = name
      open (22, file = fname, status = 'old')
      sec = secnds (73.7)
      int1 = sec
      int2 = (sec-int1) *10000
      int1 = 2* (int1/2) +1
      iseed = 2* (int2/2) +1
      do 200 i = 1, 7
      read (22, 1) a1
      write (23, 1) a1
1     format (a)
200   continue
      no = 6
      do 10 i = 1, no
      read (22, 2) e1 (i), izero, xx, x (i), y
        (i), z (i)
2     format (a2, i1, 4f18.0)
10    continue
      do 50 i = 1, no
100   dx = rad* (2.*ran (iseed) -1.)
      dy = rad* (2.*ran (iseed) -1.)
      dz = rad* (2.*ran (iseed) -1.)
      dist = sqrt (dx**2 + dy**2 + dz**2)
      if (dist.gt.rad) go to 100
      x1 (i) = x (i) + dx
      y1 (i) = y (i) + dy
      z1 (i) = z (i) + dz
      write (23, 16) e1 (i), x1 (i), y1 (i), z1
        (i)
16    format (2x, a2, ', 0, ', 3f12.5)
50    continue
      write (23, 51)
51    format (///)
      write (23, 23) rad, name
23    format (' kick size = ', f12.2, /a)
      STOP
      END
```

References

1. (a) Saunders, M. J Am Chem Soc 1987, 109, 3150; (b) Saunders, M. J Comput Chem 1989, 10, 203; (c) Saunders, M.; Krause, N. J Am Chem Soc 1990, 112, 1791; (d) Saunders, M. J Comput Chem 1991, 12, 645; (e) Chandrasekhar, J.; Saunders, M.; Jorgensen, W. L. J Comput Chem 2001, 22, 1646.
2. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, J. A. Jr.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millan, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.;. Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelly, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Baboul, A. G.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Andres, J. L.; Gonzalez, C.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A. GAUSSIAN98; Gaussian, Inc.: Pittsburgh, PA, 1998.
3. Jones, R. O. J Chem Phys 2001, 110, 5189.




sigma
Ultimaker


formlabs

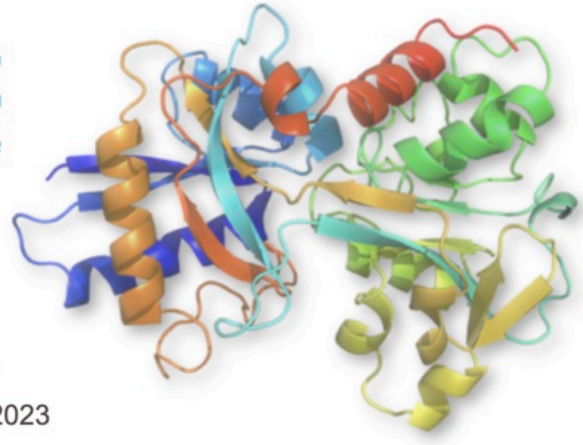
Early beginning

- Scientific project
- Equipment acquired
  - TECAN Spark
  - Opentrons OT-2

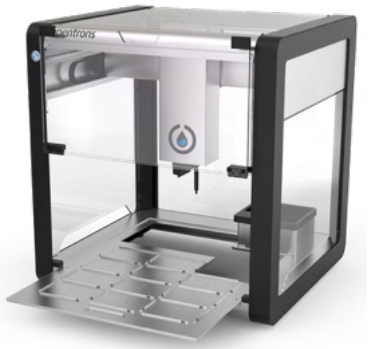
GlyMech

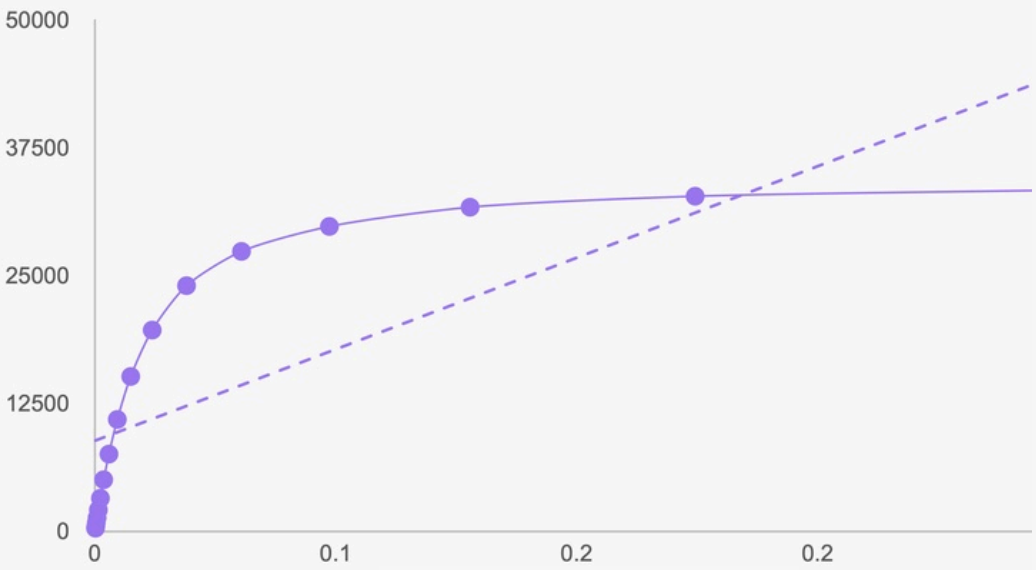
Glycosylation as a factor in the iron transport mechanism of human serum transferrin

HRZZ Croatian Science Foundation



Leader: doc. dr. sc. Tin Weitner
HRZZ project UIP-2017-05-9537
February 1, 2018 – January 31, 2023



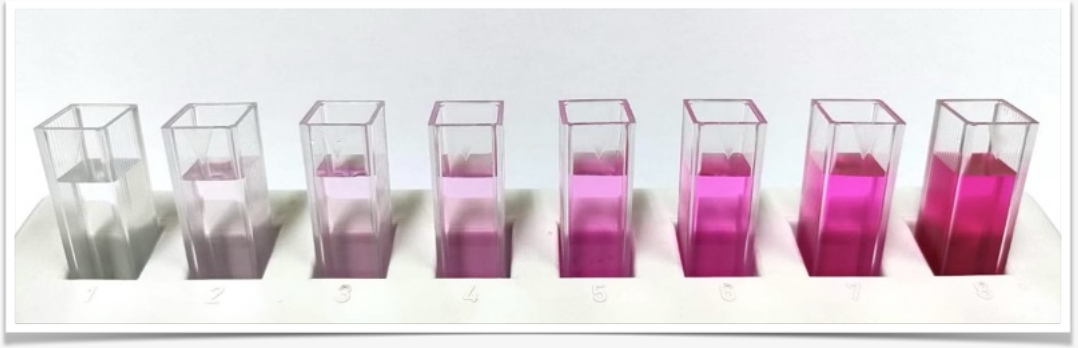


Inner filter effect

Sample has too much analyte (high concentration) or interference - emmited light is not proportional to the concentration in fluorescence spectroscopy

The Problem

FLUORESCENCE DATA IS INACCURATE IN HIGH CONCENTRATIONS



analytical chemistry

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Article

Inner Filter Effect Correction for Fluorescence Measurements in Microplates Using Variable Vertical Axis Focus

Tin Weitner,* Tomislav Friganović, and Davor Šakić

Cite This: *Anal. Chem.* 2022, 94, 7107−7114

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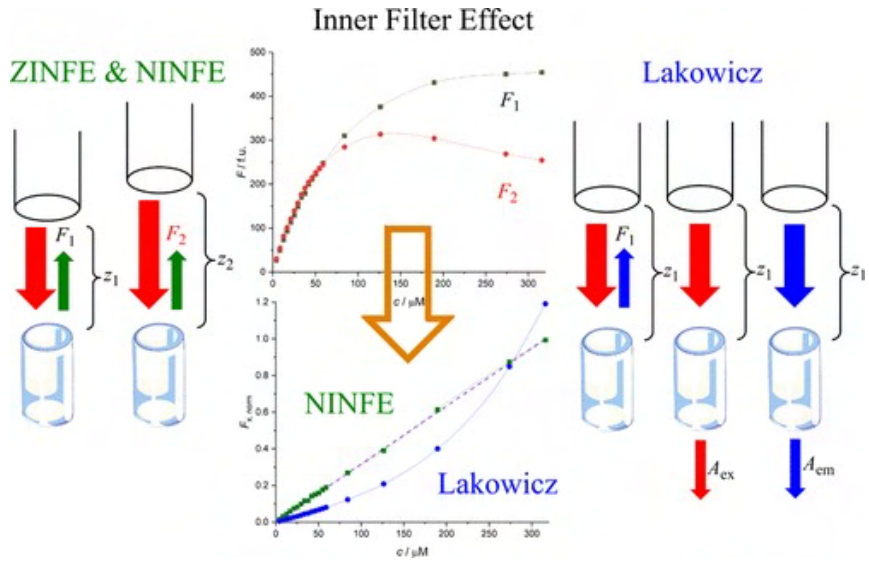
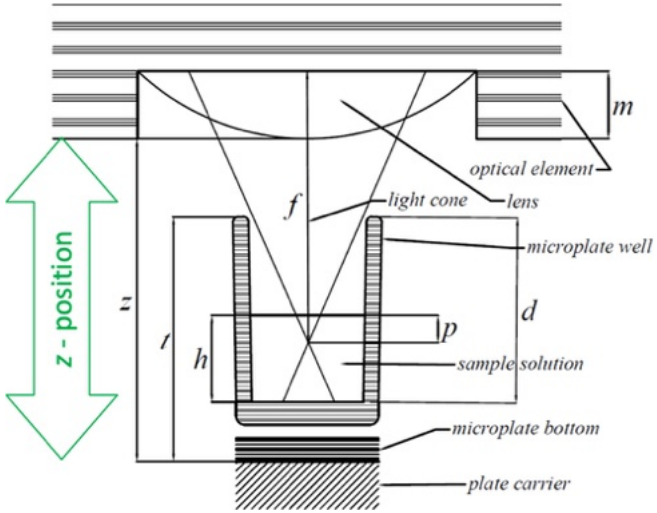
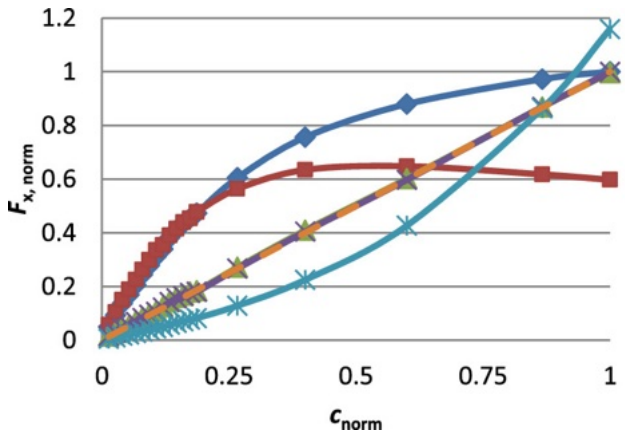
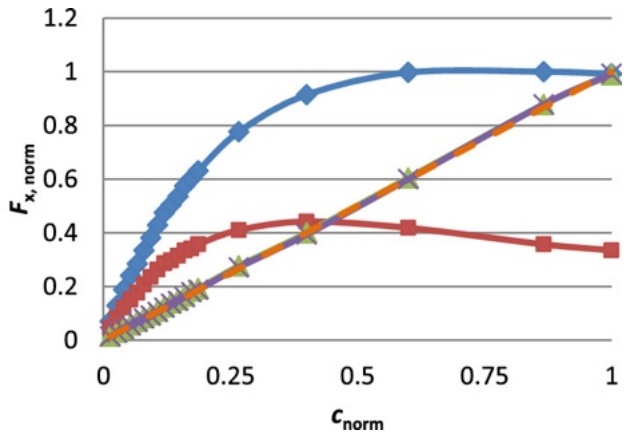








Ključni datumi i aktivnosti

19. 10. otvaranje prijava za znanstvenike i tvrtke

27. 11. – 28. 1. spajanje prijavljenih znanstvenika i tvrtki

28. 1. kraj prijava za znanstvenike i tvrtke

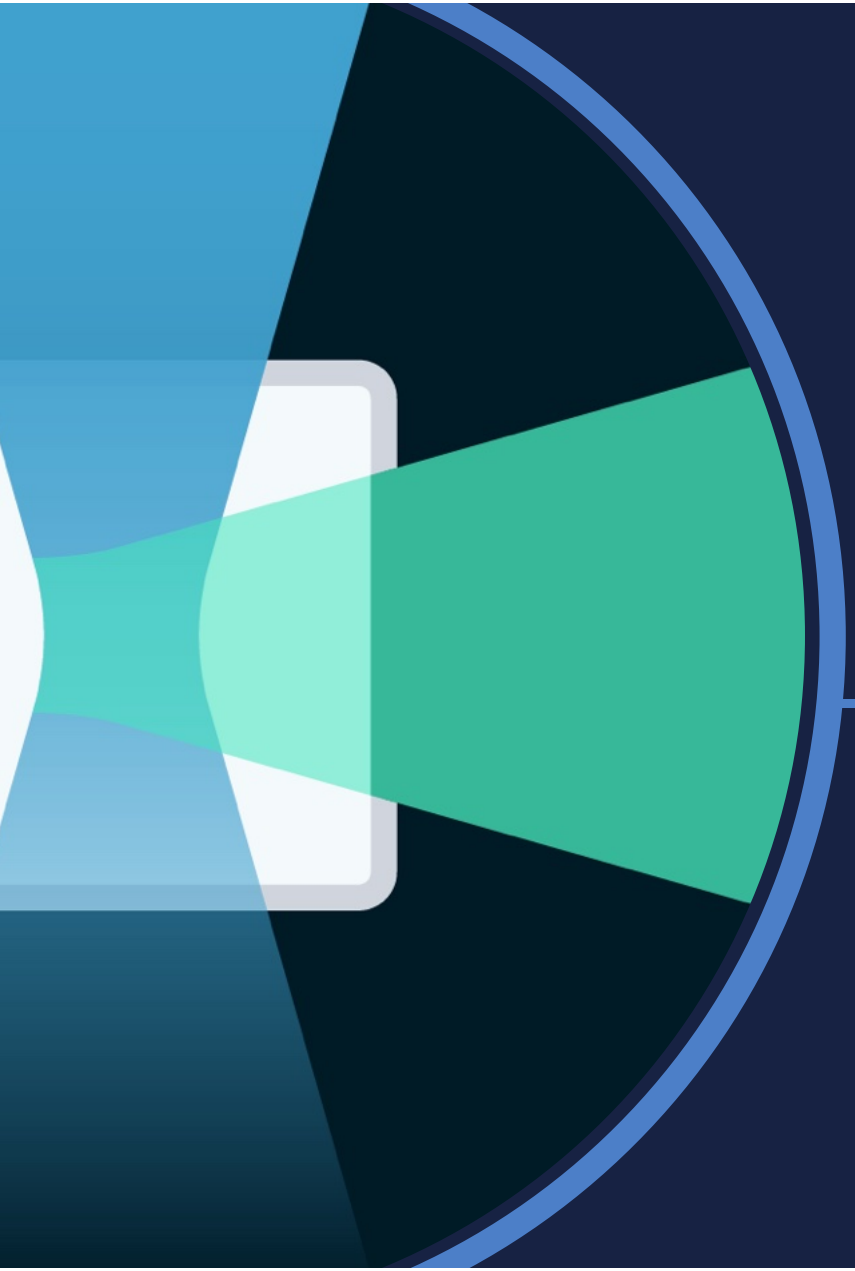
29. 1. – 4. 2. obavještavanje odabranih sudionika

8. 2. predstavljanje projekta svim odabranim tvrtkama

14. – 15. 2. dvodnevni događaj SCINERGY '24

1. **dan**: *speed-dating* odabranih znanstvenika i tvrtki, predstavljanja uspješnih suradnji znanstveno-istraživačkih institucija i gospodarstva te prilika za financiranje takvih suradnji
2. **dan**: nastavak upoznavanja i razgovora o potencijalnim suradnjama znanstvenika i tvrtki kroz vođenu radionicu

16. 2. – 30. 4. vođeni sastanci za uspostavljanje suradnji, edukacija, validacija ideja, pravna podrška, povezivanje s prilikama za financiranje suradnje



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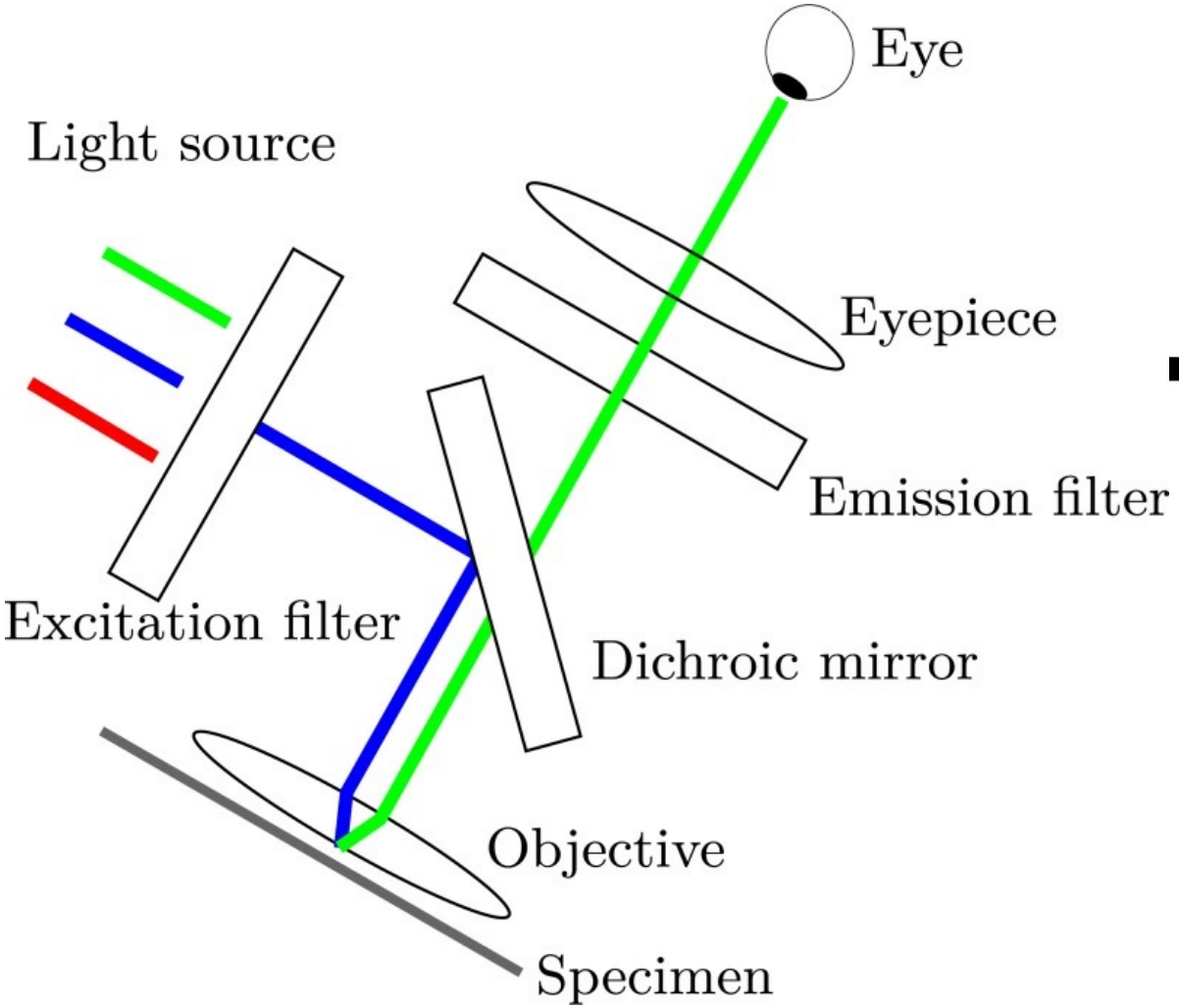
Eye
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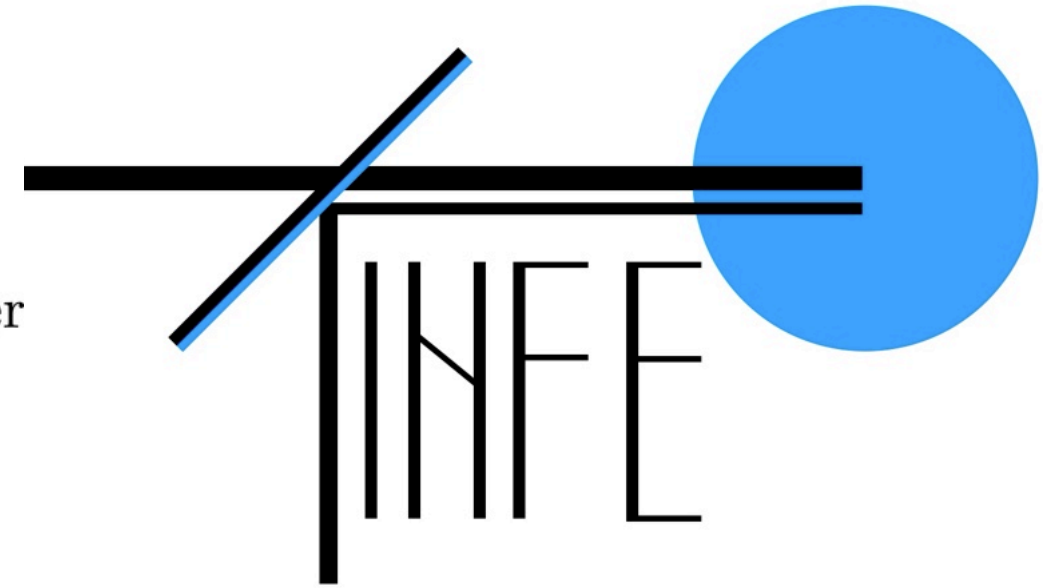
Eyepiece
Emission filter
Excitation filter
Dichroic mirror
Objective
Specimen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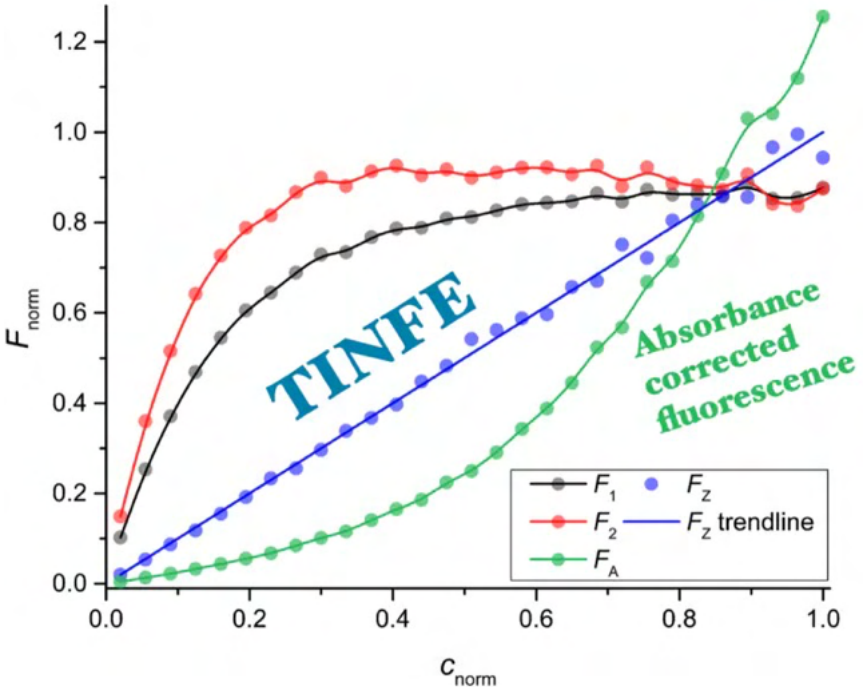
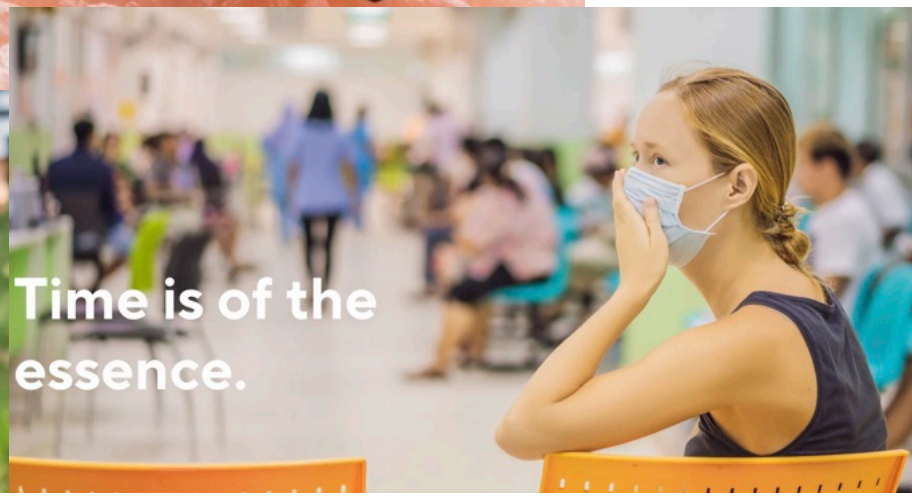

TINFE
Absorbance corrected fluorescence
F_1
F_z
F_2
F_z trendline
F_A
F_{norm}
c_{norm}
0.0
0.2
0.4
0.6
0.8
1.0
1.2


Do you have
time to waste?


Ticks happen
Time is of the
essence.


Time is of the
essence.


Time is of the
essence.

Steps in analysis

AQUISITION

PREPARATION

TRANSFER

MEASUREMENT

Sample challenges

Unknown concentrations, interferences, limited ranges, **small volumes.**

Resource constraints

Limited personnel availability, extended turnaround times, **less profit**.

Operational challenges

Time-intensive prep, costly reagents, high-throughput needs, specific labware, **high cost**.

TINFE

Measure twice, analyse once.

- Correcting nonlinear response of emission spectra
- Two measurements at different settings
- Advanced signal processing on two datasets
- Reliable data with increased accuracy, precision and linear range


NUCLEUS
DEMO DAY
July 4th, 2024
Davor Šakić
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4.7.2024.
HUB385
Strossmayerova 6
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brand
insight
POTROŠAČI

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Biochemical test

HEART TROPONIN
D-DIMERS
LIPOPROTEIN A

Heart stroke symptoms

Chest discomfort
Lightheadedness & nausea
Left arm and shoulder pain
Cold sweat
Shortness of breath
Jaw, neck or back pain

Golden hour

Critical 60-minute window
Swift medical intervention
improves the outcome

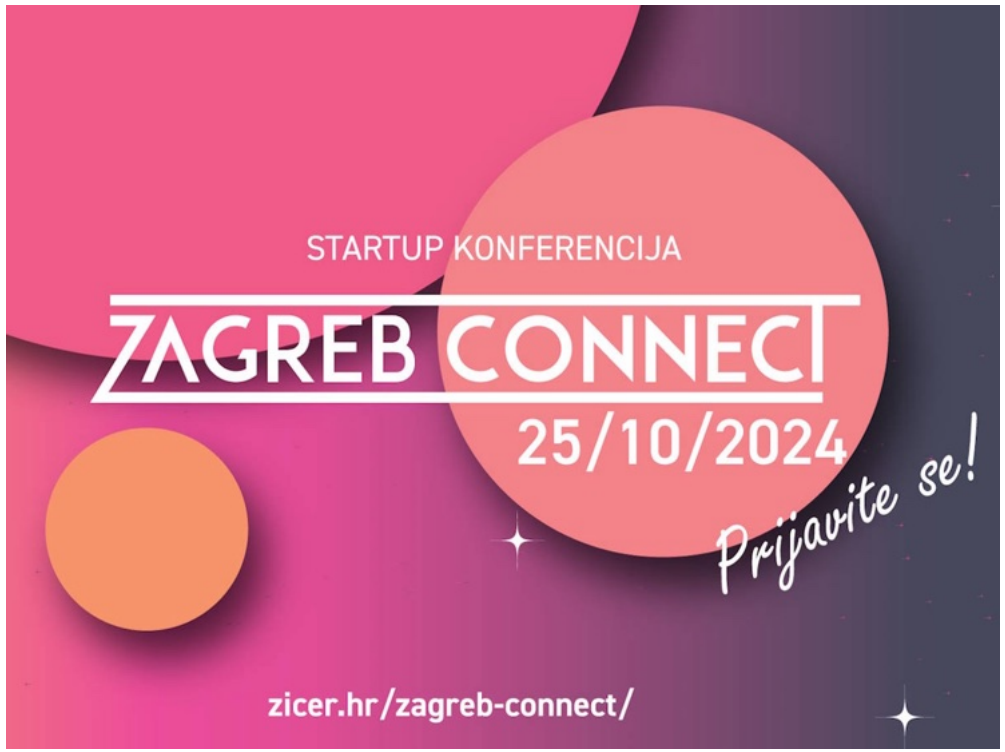
» Relevance

TINFE

As my time ticks down

Let’s save someone else’s time together

»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Semi-Finals - October 21, 2024.
Finals - October 29, 2024.
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Ulica Filipa Vukasovića 1, Zagreb
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2nd Prize:
5.000€ (2 positions)
3rd Prize:
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Innovation & Investment
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Zagreb School of Economics and Management
Eureka International Innovation and Entrepreneurship Competition
Startup Competition
CONGRATULATIONS!
Award Ceremony
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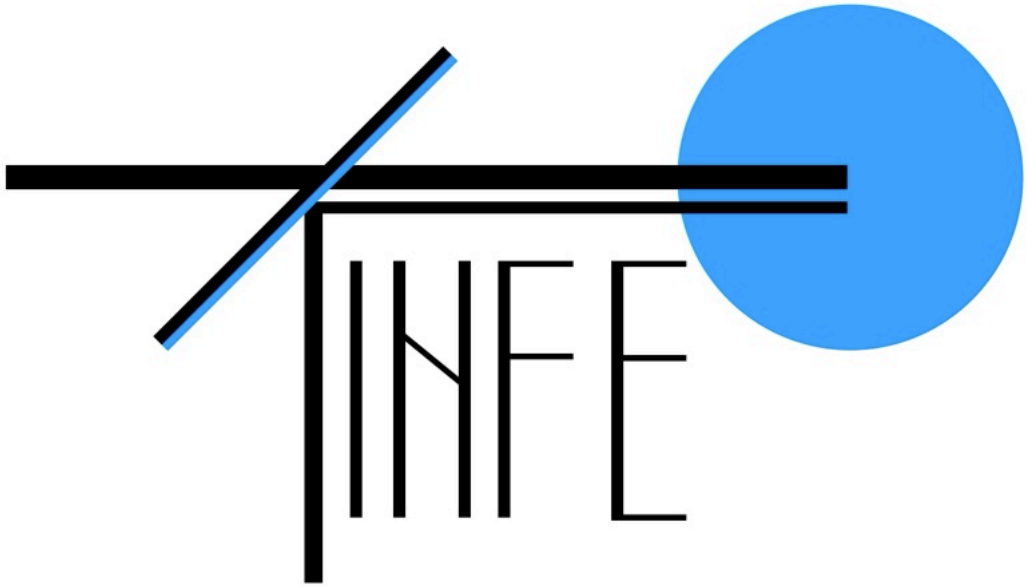
BRONČANO TESLINO JAJ
VIDI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Professional

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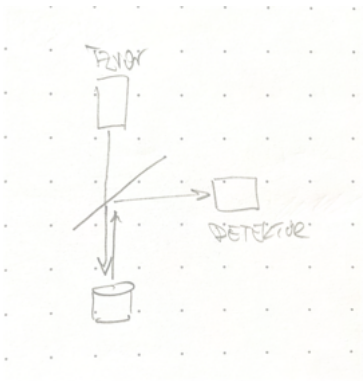

Hw+Sw

Fluorescent
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Ušteda
vremena

Resource
Efficency

Scientific

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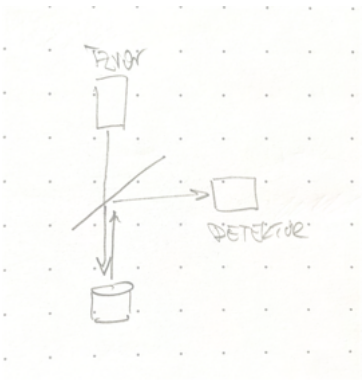
#1



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Hw+Sw

Fluorescent
spectroscopy

Ušteda
vremena

Resource
Efficency

Scientific

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Input for TINFE

CALIBRATION

Choose File no file selected

After selecting file, please be patient while results are generated.
Before uploading a new calibration dataset please click the 'START AGAIN' button below to clear previously uploaded values. For full report with all calculated values please select 'DOWNLOAD RESULTS' checkbox below.

GEOMETRIC PARAMETER:

0.020593

Default for Tecan Spark M10 microplate reader and 96-well, black, flat bottom microplates (cat. no. 30122298, Tecan, Austria).

READOUT

Choose File no file selected

- [ ] LINEARITY OF RAW DATA
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- [x] DOWNLOAD GRAPHS

START AGAIN

Total INner Filter Effect Corrector - TINFE

INFO & USER GUIDE

Introduction to TINFE

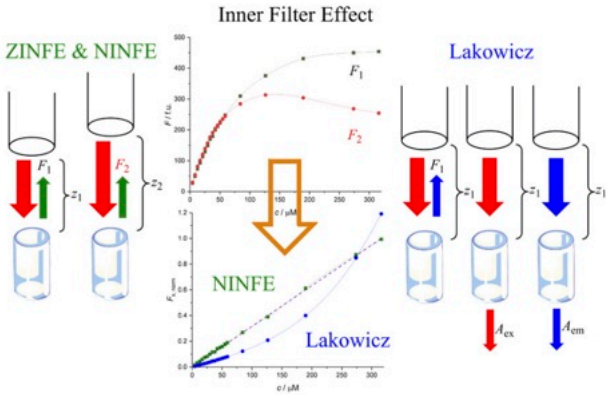
Friganović, Šakić, Weitner, 2020.-2024.

Corrector function to eliminate inner filter effect for fluorescence measurements in microplates using variable z-positions.

For more information please consult published paper:

Weitner, T.; Friganović, T.; Šakić, D.
Inner Filter Effect Correction for Fluorescence Measurements in Microplates Using Variable Vertical Axis Focus.
Analytical Chemistry, 2022. doi:10.1021/acs.analchem.2c01031

Raw data can be found here: doi:10.5281/zenodo.5849302



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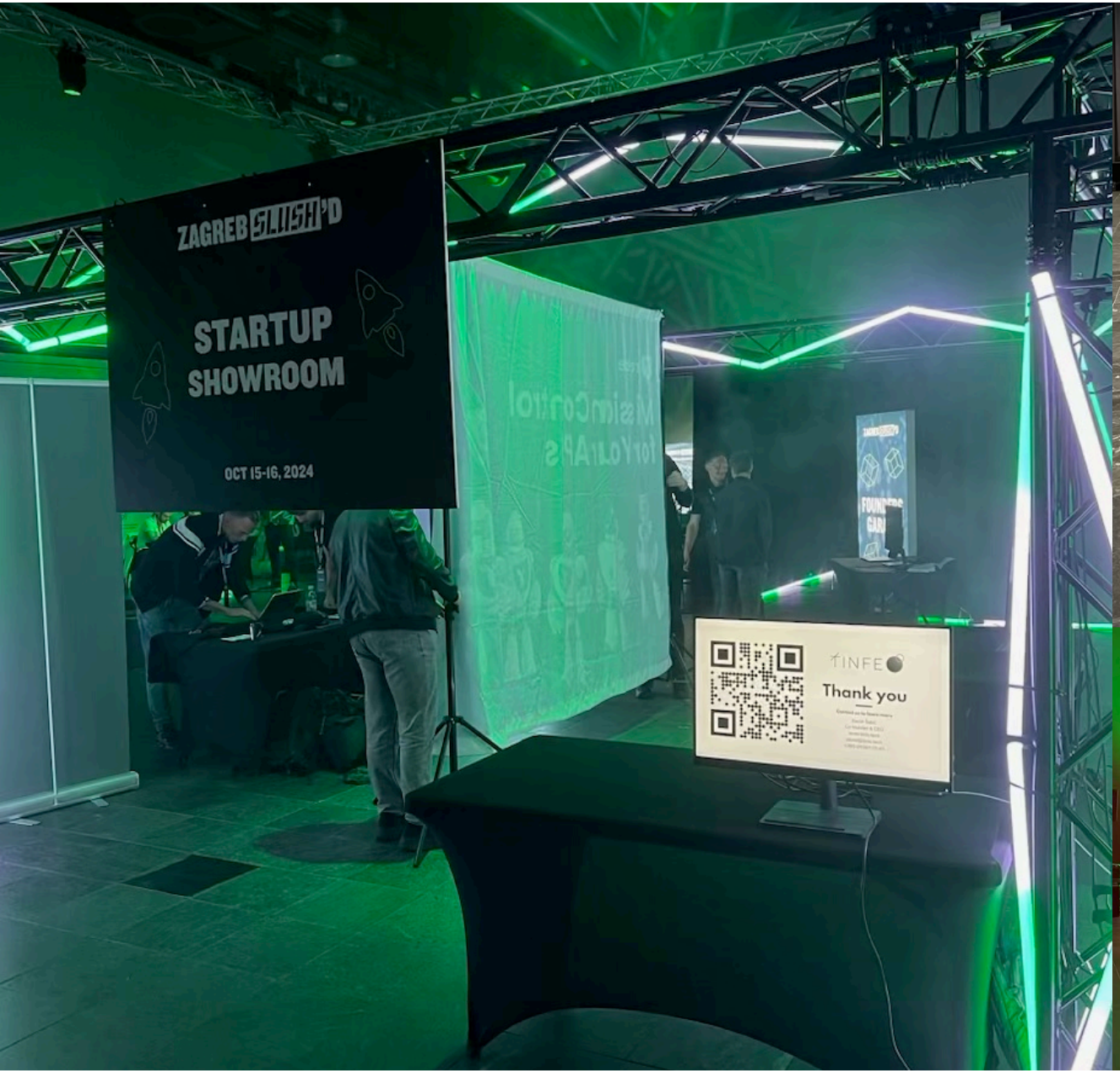
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SHOWROOM
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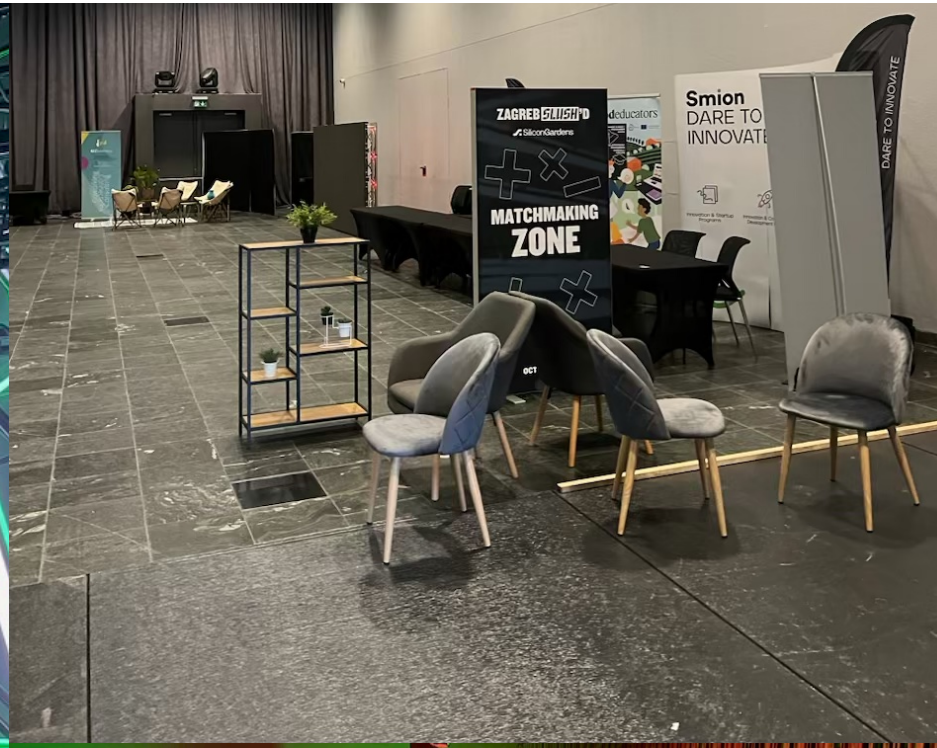
Thank you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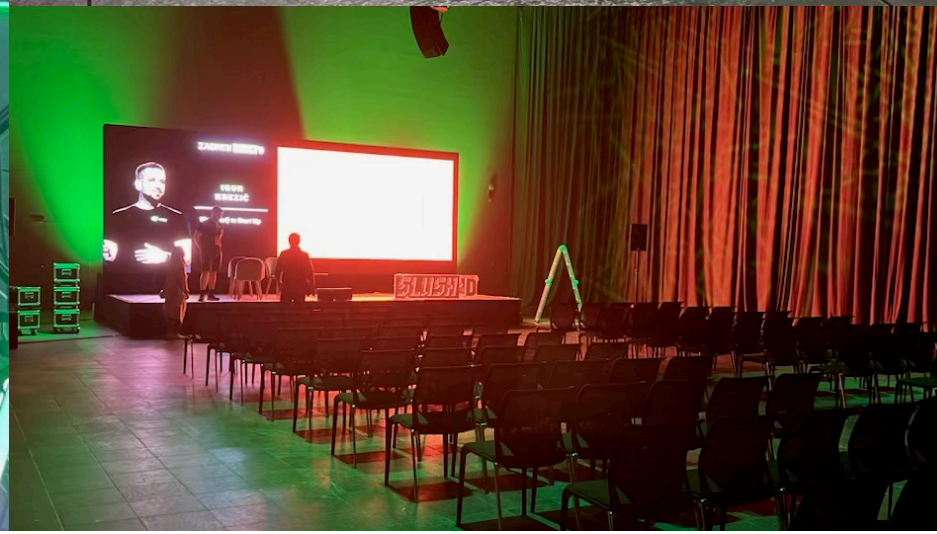
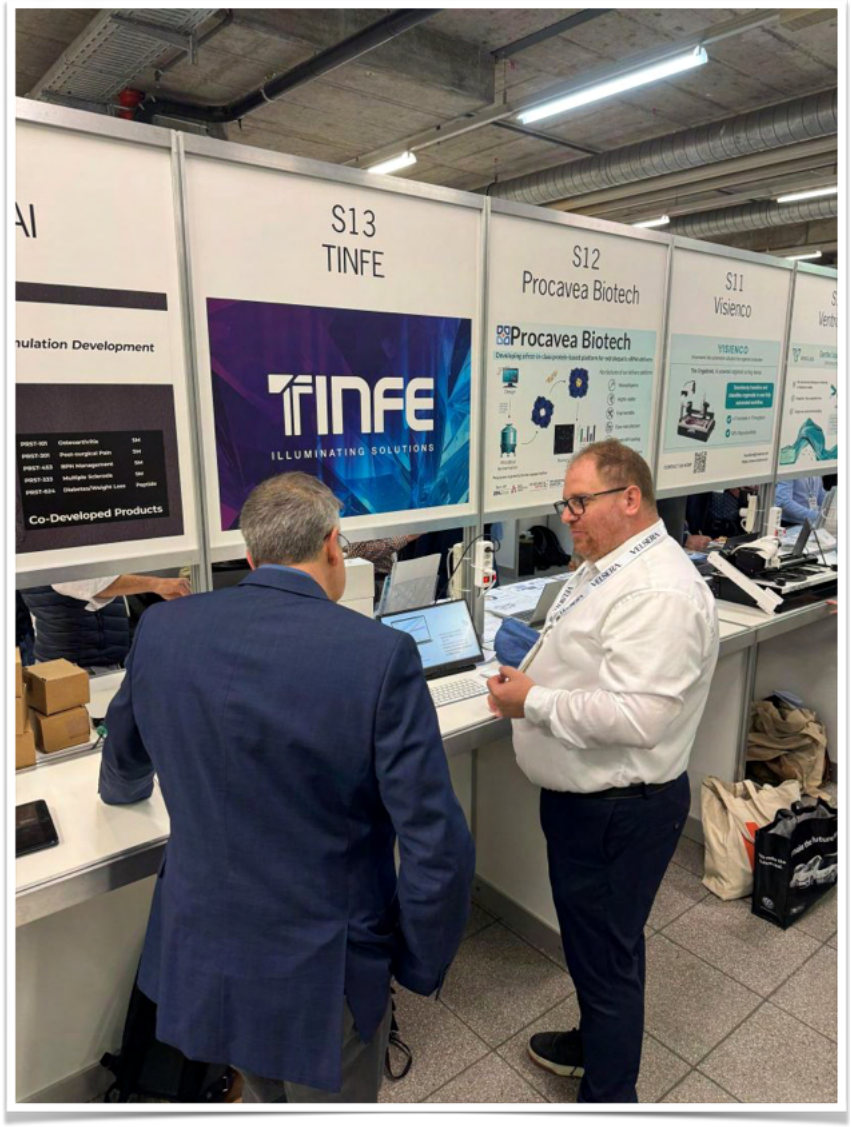

SLUSH'D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Who? The top 10 Croatian deep-tech startups
Where? Royal Academy of Engineering, Sir Kirby Laing Room
When? January 13th - 15th, 2025
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WHAT IT TAKES TO GET RESULTS


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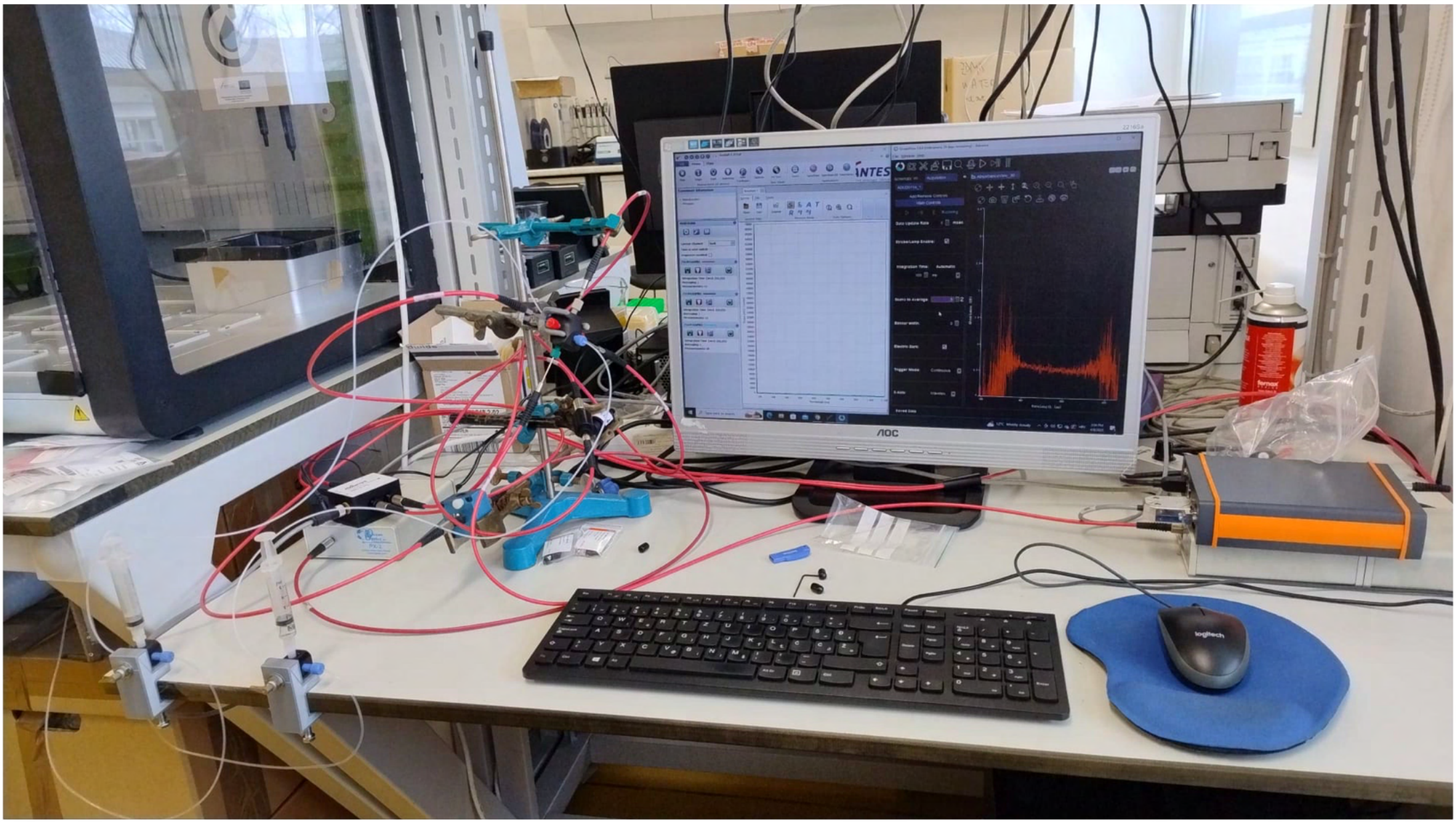
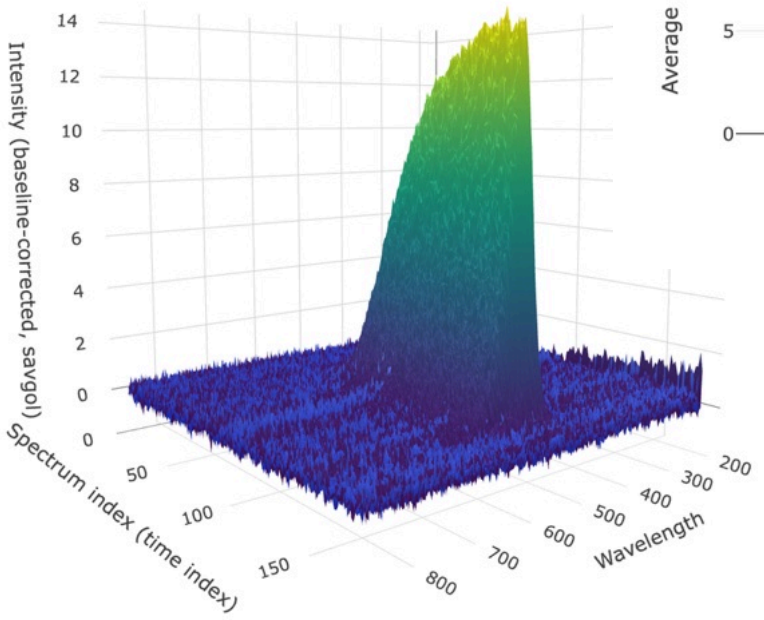
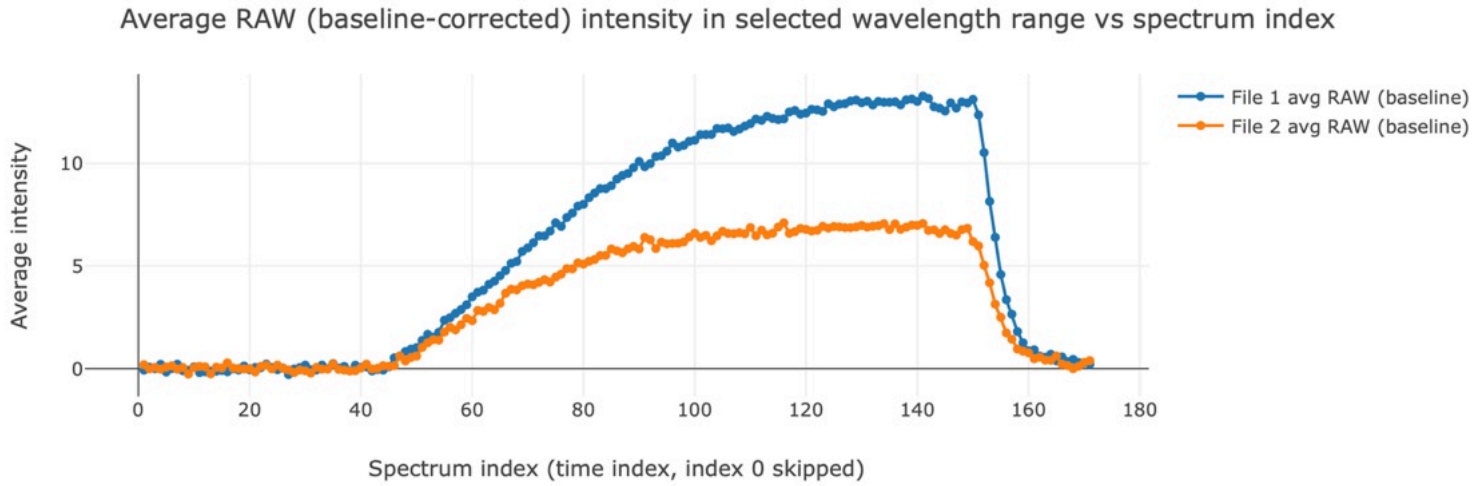
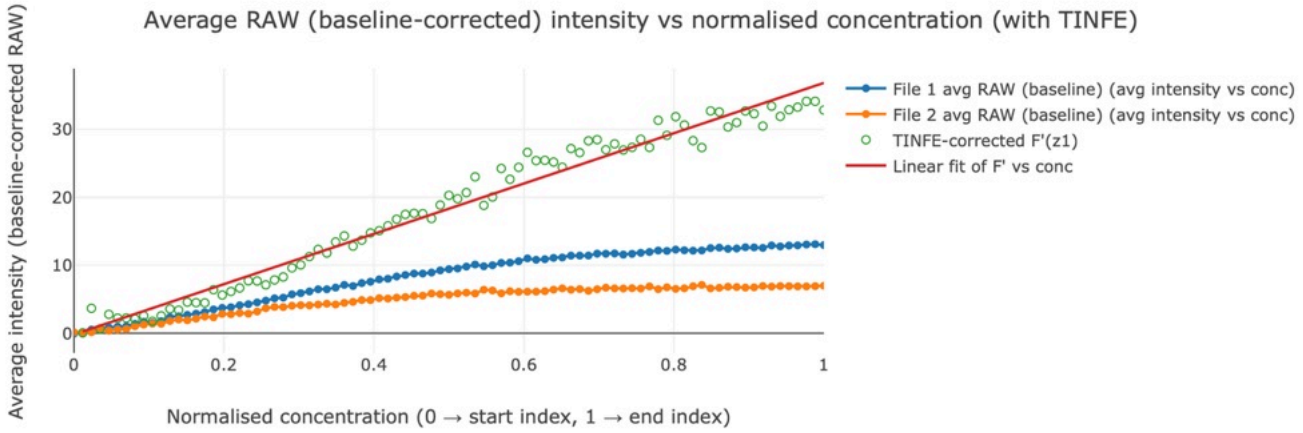
SPARK
TECAN


AOC
logitech







TESTING

TINFE correction (using first two fluorescence traces):
F'(c) = F(z1) · (F(z1)/F(z2))^n
Best n ≈ 1.500
Linear fit: F'(c) = a·c + b
a (slope) ≈ 3.698832e+1
b (intercept) ≈ -1.830346e-1
R^2 ≈ 0.974181
Points used = 86


European Commission
#HorizonEU
HORIZON EUROPE
THE EU
RESEARCH & INNOVATION
PROGRAMME
2021 – 2027
LUMP SUM FUNDING:
WHAT DO I NEED TO KNOW?
24 JUNE 2024
V3.0
A GUIDE FOR PARTICIPANTS
EUROPEAN COMMISSION, DG RTD
Common Implementation Centre
Common Service for Business Processes
Research and Innovation


logitech
KAFFEREP
VINTERSAGA
Ginger thins
IKEA
300 g
KAFFEREP
350 g
IKEA
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SEAL OF
EXCELLENCE
European Commission
European Commission
Horizon Europe
The project proposal
101309842 — BRIGHT
"Digital Platform for Fluorescence Signal Correction and Data Integrity"
submitted under the Horizon Europe call
HORIZON-WIDERA-2025-02-ACCESS-01 — EIC pre-accelerator - Widening
by
TINFE HTS llc
following evaluation by an international panel of independent experts
was recognised as a high-quality project proposal
in a highly competitive evaluation process
but could not receive funding due to budgetary constraints and is therefore
recommended by the European Commission for funding by other sources.

DIGITAL, INNOVATION, AND GREEN TECHNOLOGY PROJECT (DIGIT PROJECT)

DIGIT
DIGITAL, INNOVATION, AND GREEN TECHNOLOGY PROJECT

REPUBLIKA HRVATSKA
Ministry of Science, Education and Youth

THE WORLD BANK
IBRD • IDA | WORLD BANK GROUP

Cost of an Error

ONE SMALL QC ERROR CAN DESTROY A SIX-FIGURE BATCH IN A SINGLE AFTERNOON.

1. Premium Production

A single batch of high-end whiskey/tequila:
€180k–€300k in production value per batch.
A single inaccurate **QC** assay (contaminant, alcohol % drift, color/phenolic reading error) can force:

- Reprocessing
- Downgrading to a cheaper product
- Full batch disposal

Cost of an Error

IN BIOLOGICS, ONE ERROR CAN WIPE OUT €20+ MILLION INSTANTLY.

2. Biological Pharmaceuticals (mAb production)

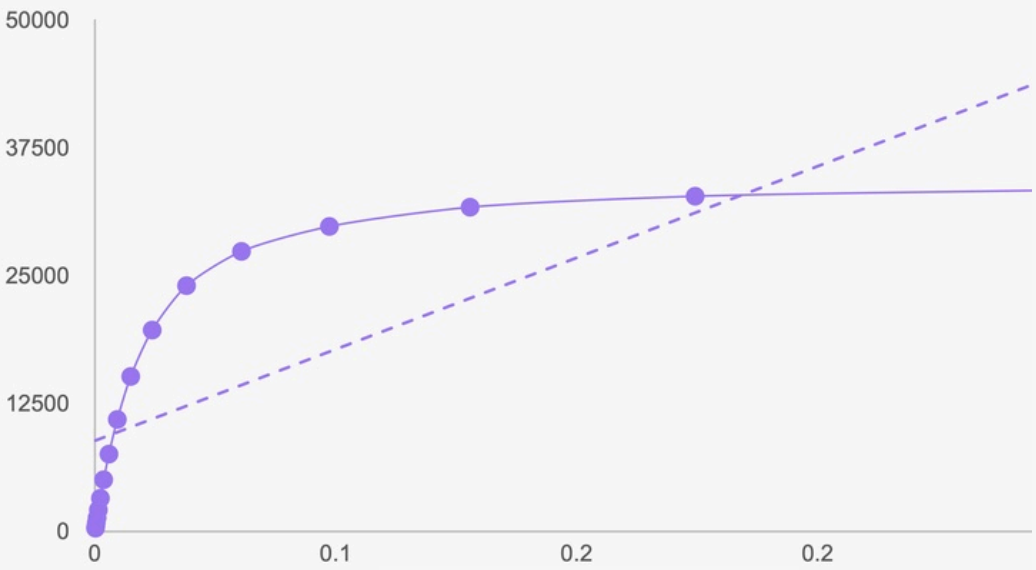
A 10,000 L bioreactor run for antibody production is **€1.5M–€9M** in manufacturing cost per batch.
If a QC measurement fails, the batch may be unsafe for release → remediation or full product **recall.**
Recent example: **ALTUVIIIO** (antihemophilic factor, recombinant) lot EY0330 recall ~ **€20M**

Cost of an Error

A €10 TEST CAN EASILY TRIGGER €1,000+ IN DOWNSTREAM COSTS.

3. Hospital and Patient Care

A crucial lab test (e.g. troponin):
Test cost: €5–€25, but important for decision making.
Turn-around-time is **3 hours**, and other analyses need to be performed.
If test results are unclear or repeated, delay adds **€300–€1k+** per day per patient in hospital stay costs.
Small diagnostic errors → big operational losses.

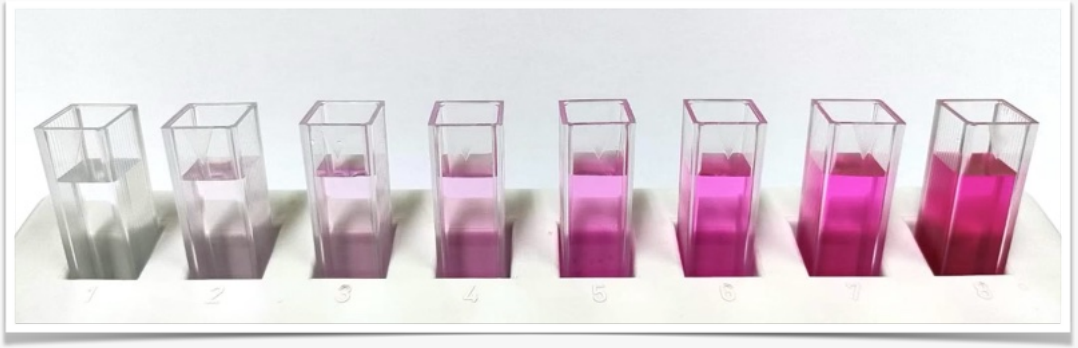


Inner filter effect

Sample has too much analyte (high concentration) or interference - emmited light is not proportional to the concentration in fluorescence spectroscopy

The Problem

FLUORESCENCE DATA IS INACCURATE IN HIGH CONCENTRATIONS



Inputs

ANNUAL NUMBER OF PLATES RUN

260

Default: 1 plate per workday

FAILURE RATE DUE TO IFE (%)

15

MATERIAL COST PER PLATE (€)

192

Default: 96 wells × €2 per well

TIME TO RE-RUN A PLATE (HOURS)

2.5

TECHNICIAN HOURLY COST (€)

25

TINFE EFFICIENCY (% OF IFE RE-RUNS ELIMINATED)

80

Estimated annual impact

COST SAVED (MATERIAL ONLY)

€5,990

COST SAVED (TIME TO RE-RUN)

€1,950

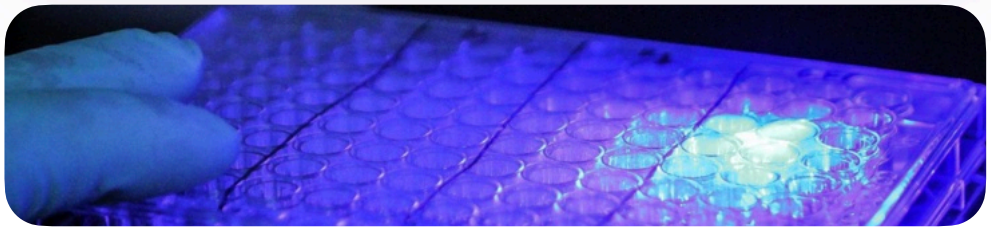
TOTAL COST SAVED

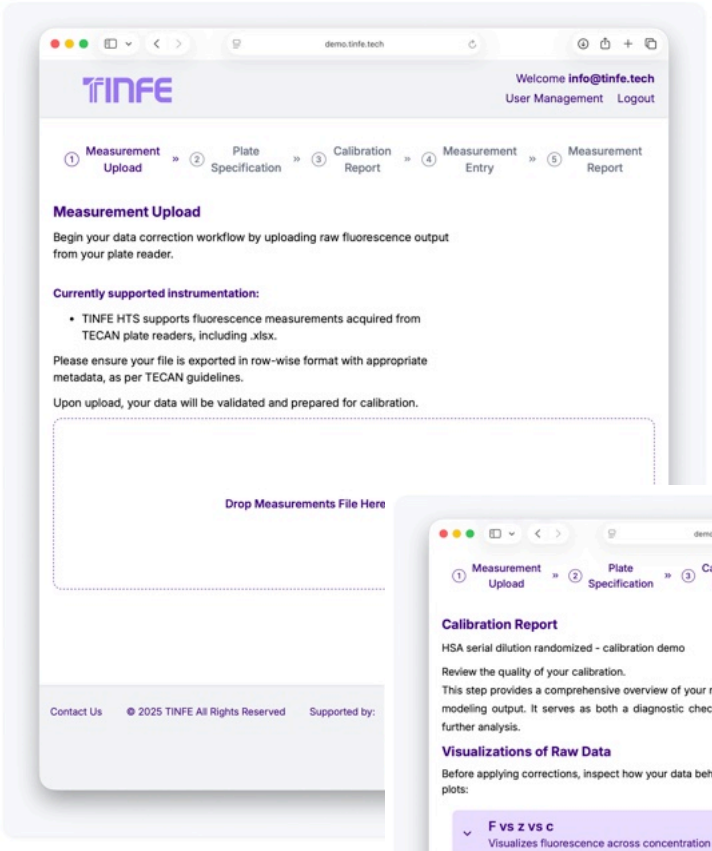
€7,940

TOTAL TIME SAVED

78 hrs

- ✓ Removes avoidable reruns caused by IFE-related distortion
- ✓ Reduces technician time spent on manual dilution and repeat analysis
- ✓ Preserves throughput while improving data quality

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TINFE
Welcome info@tinfe.tech
User Management Logout
1 Measurement Upload » 2 Plate Specification » 3 Calibration Report » 4 Measurement Entry » 5 Measurement Report
Measurement Upload
Begin your data correction workflow by uploading raw fluorescence output from your plate reader.
Currently supported instrumentation:
• TINFE HTS supports fluorescence measurements acquired from TECAN plate readers, including .xlsx.
Please ensure your file is exported in row-wise format with appropriate metadata, as per TECAN guidelines.
Upon upload, your data will be validated and prepared for calibration.
Drop Measurements File Here
Contact Us
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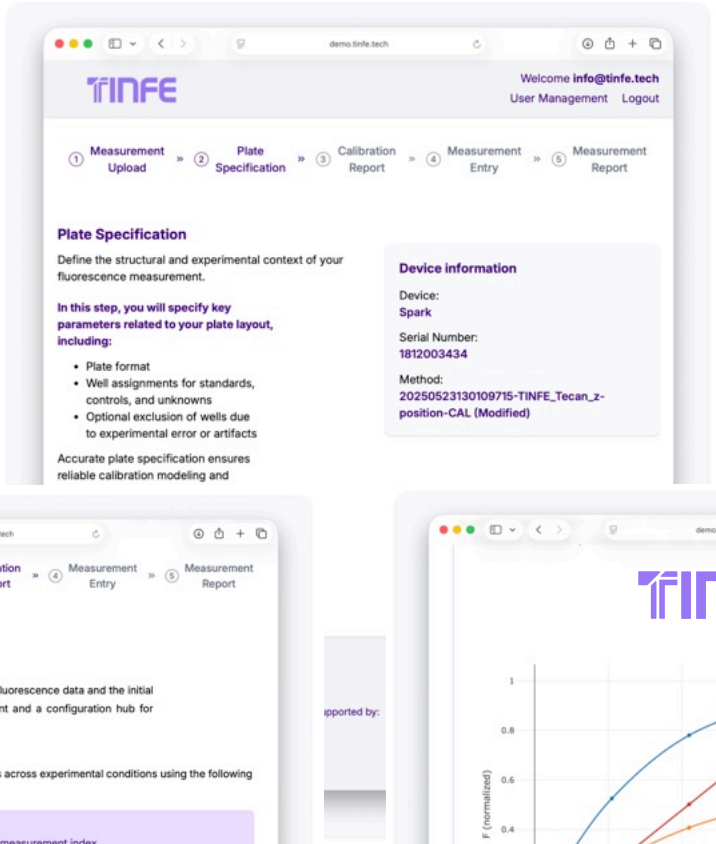
Supported by: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TINFE
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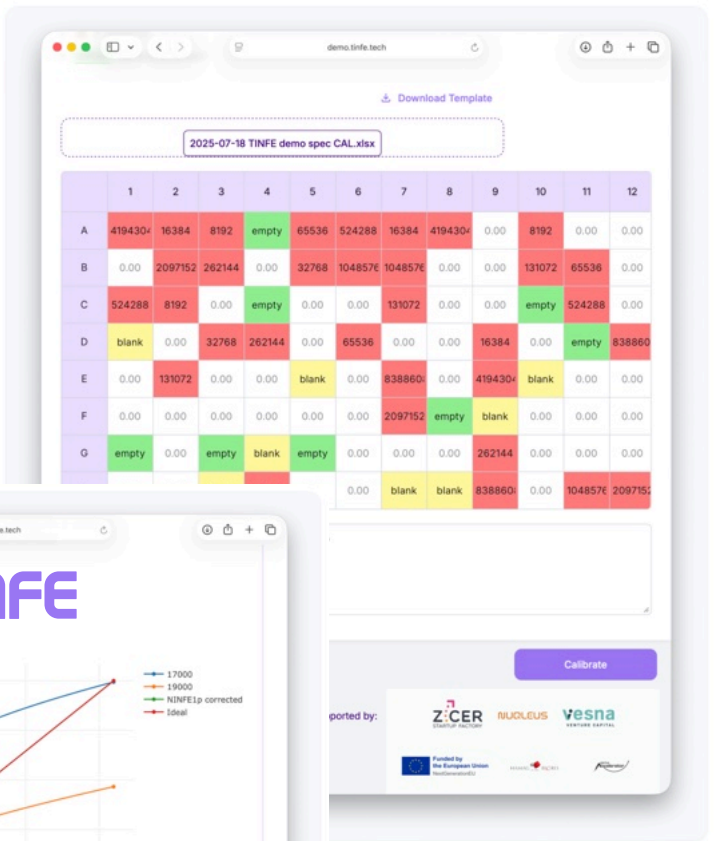
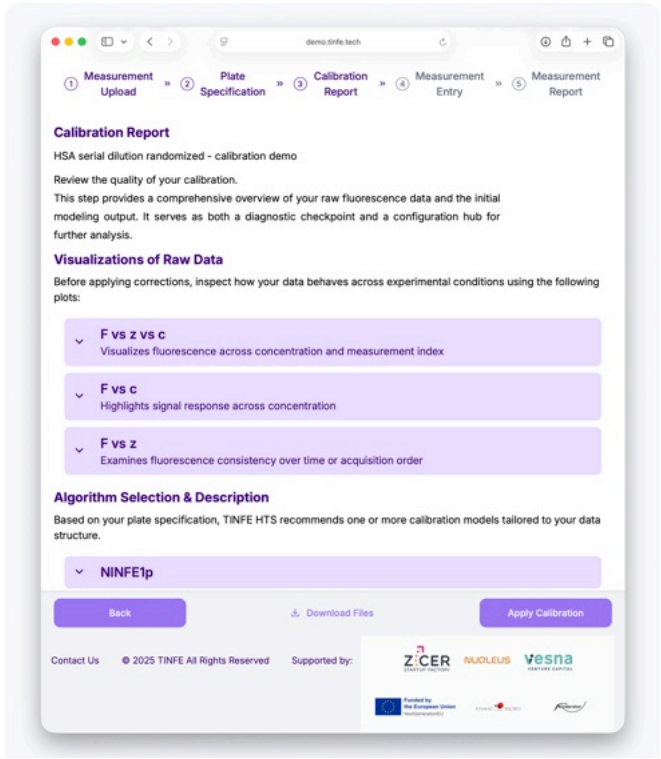
1 Measurement Upload » 2 Plate Specification » 3 Calibration Report » 4 Measurement Entry » 5 Measurement Report
Plate Specification
Define the structural and experimental context of your fluorescence measurement.
In this step, you will specify key parameters related to your plate layout, including:
• Plate format
• Well assignments for standards, controls, and unknowns
• Optional exclusion of wells due to experimental error or artifacts
Accurate plate specification ensures reliable calibration modeling and
Device information
Device:
Spark
Serial Number:
1812003434
Method:
20250523130109715-TINFE_Tecan_z-position-CAL (Modified)


demo.tinfe.tech
Download Template
2025-07-18 TINFE demo spec CAL.xlsx
Calibrate
Supported by:


demo.tinfe.tech
1 Measurement Upload » 2 Plate Specification » 3 Calibration Report » 4 Measurement Entry » 5 Measurement Report
Calibration Report
HSA serial dilution randomized - calibration demo
Review the quality of your calibration.
This step provides a comprehensive overview of your raw fluorescence data and the initial modeling output. It serves as both a diagnostic checkpoint and a configuration hub for further analysis.
Visualizations of Raw Data
Before applying corrections, inspect how your data behaves across experimental conditions using the following plots:
F vs z vs c
Visualizes fluorescence across concentration and measurement index
F vs c
Highlights signal response across concentration
F vs z
Examines fluorescence consistency over time or acquisition order
Algorithm Selection & Description
Based on your plate specification, TINFE HTS recommends one or more calibration models tailored to your data structure.
NINFE1p
Back
Download Files
Apply Calibration
Contact Us
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Supported by:


demo.tinfe.tech
TINFE
17000
19000
NINFE1p corrected
Ideal
F (normalized)
c
Deviation from ideal line
Back
Download Files
Apply Calibration
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TAM (All global ICP labs + add-on sales)

€ 1.2 Billion pa

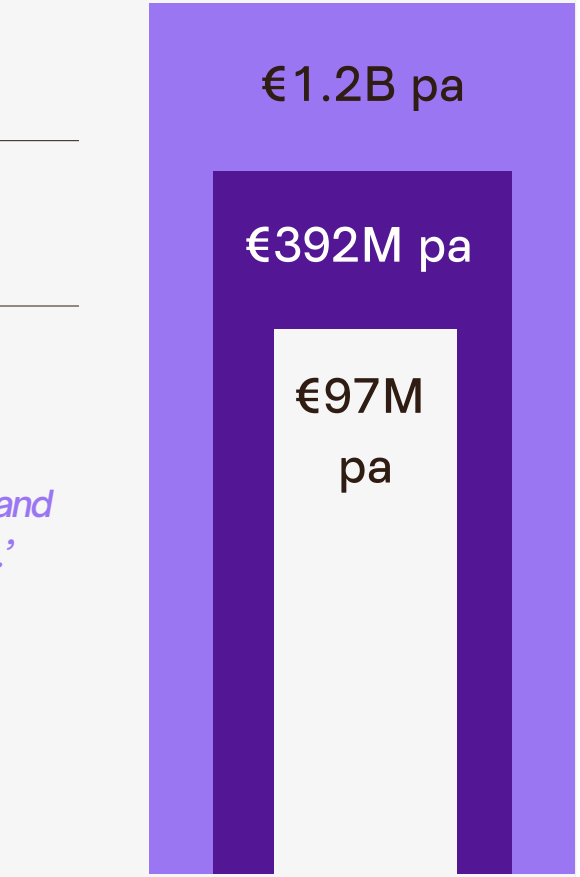
SAM (All Euro ICP labs + add-on sales)

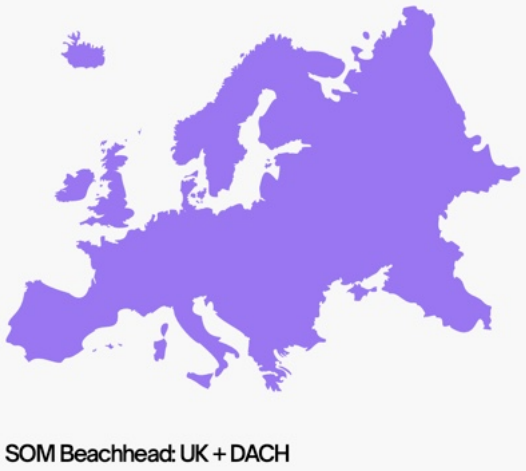
€ 392 Million pa

SOM (4-year sales projection)

€ 97 Million pa

Life sciences are rapidly expanding, and fluorescence is the lab's 'workhorse.'





SOM Beachhead: UK + DACH

Competition

OR FUTURE PARTNERS?

BMG LABTECH
The Microplate Reader Company

Agilent

TECAN.

MOLECULAR DEVICES

HORIBA

revvity

BECKMAN COULTER

Roche

Abbott

SIEMENS Healthineers

Industry Pilots

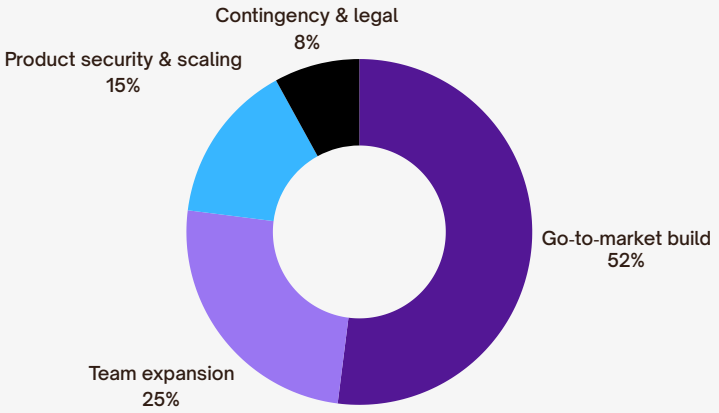
3+ collaboration with food industry, contact research laboratories, and strategic partner for real case scenarios

Reduction in Re-runs

80% reduction in assay reruns, directly translating to significant savings in time, reagents, and labor costs

Funds Secured

€100k in non-dilutive innovation funding from European and national grant programs + VC backed PoC grant



Traction Achieved

WHAT IS NEXT

€ 500k
EIC WIDERA call

€ 700k
pre-seed round

NUQLEUS vesna VENTURE CAPITAL ZICER ZAGREB INNOVATION CENTRE startup Akcelerator Funded by the European Union NextGenerationEU HAMAG BICRO