

AIWizard™

METTLER TOLEDO

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Thermal Analysis

A group of techniques in which a physical property of a substance is measured as a function of temperature whilst the substance is subjected to a controlled temperature program



ICTAC

International Confederation for Thermal Analysis and Calorimetry

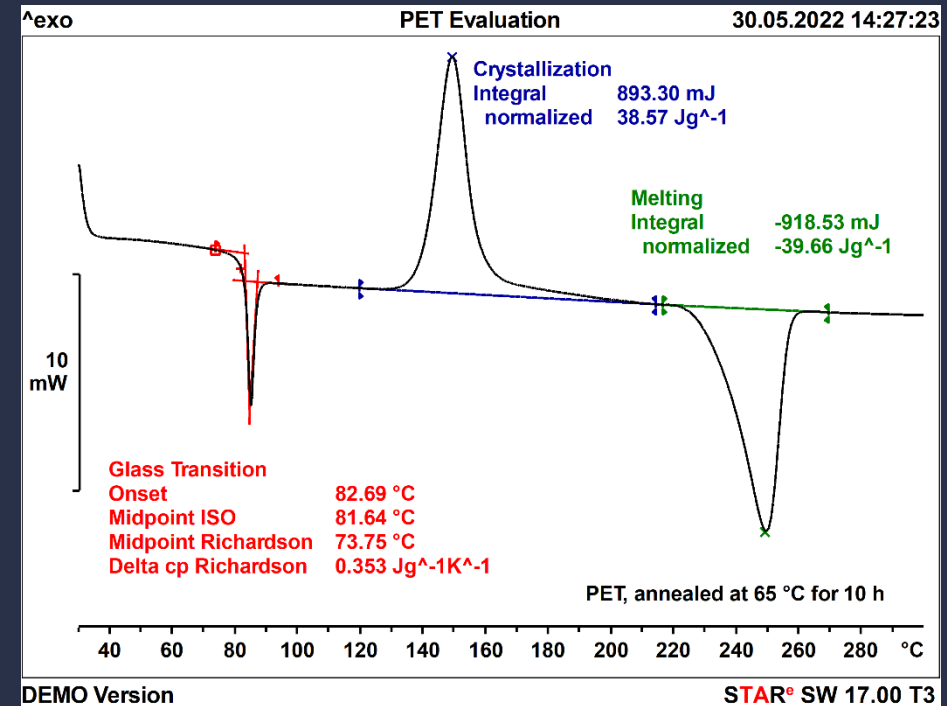
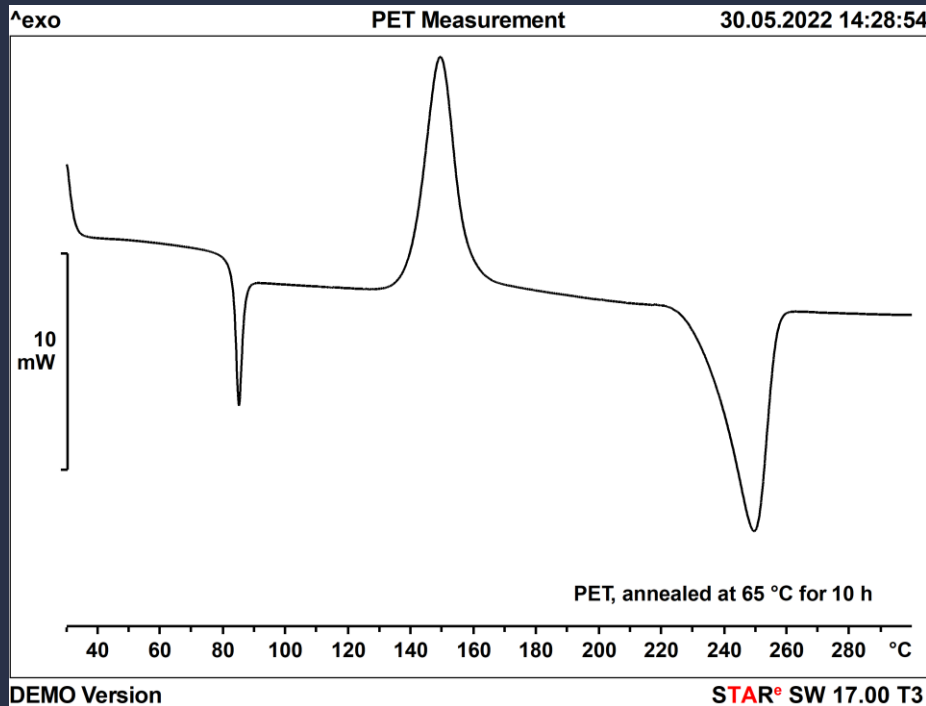
Evaluation



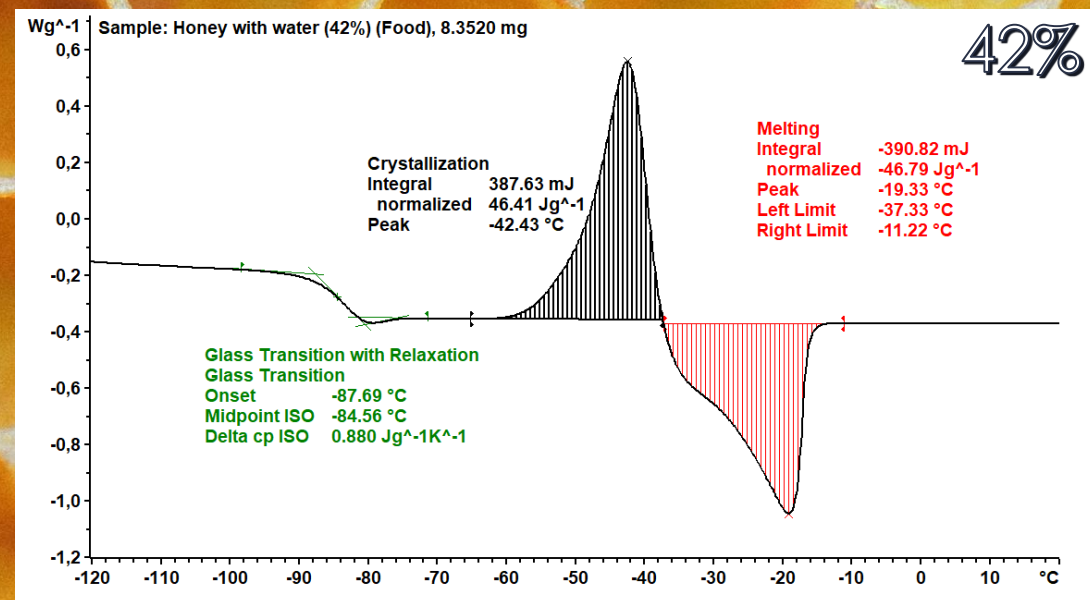
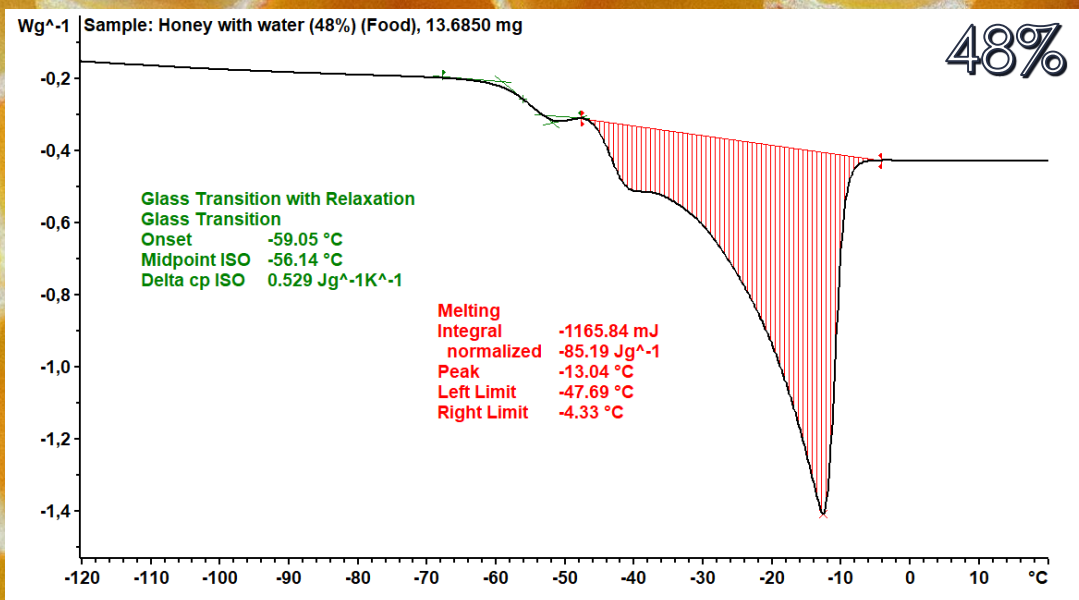
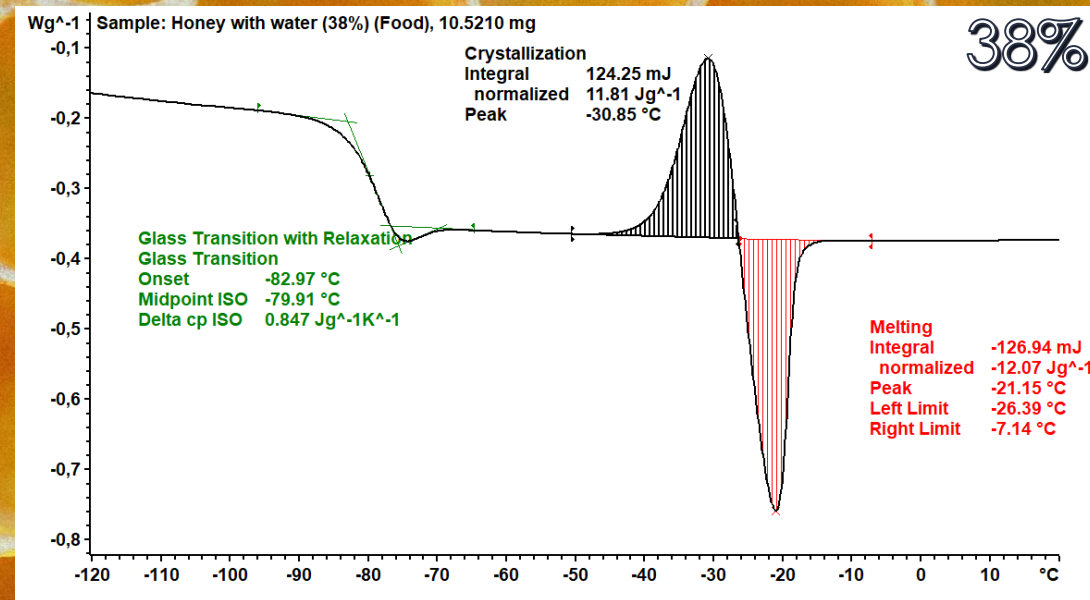
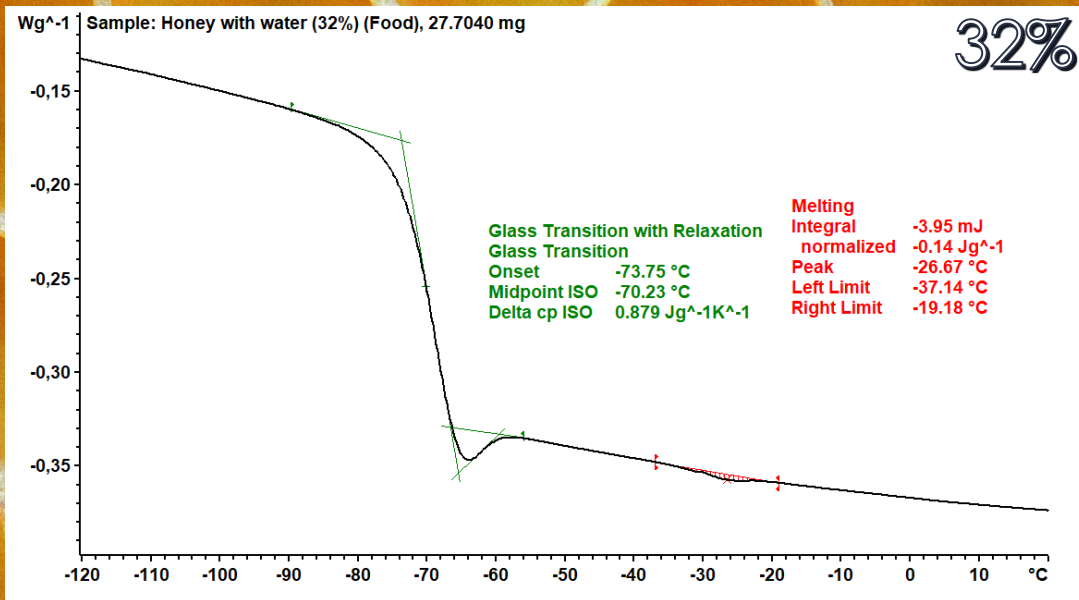
Many users struggle with:

- Effect or artifact?
- What effect is it?
- Begin and end of an effect?

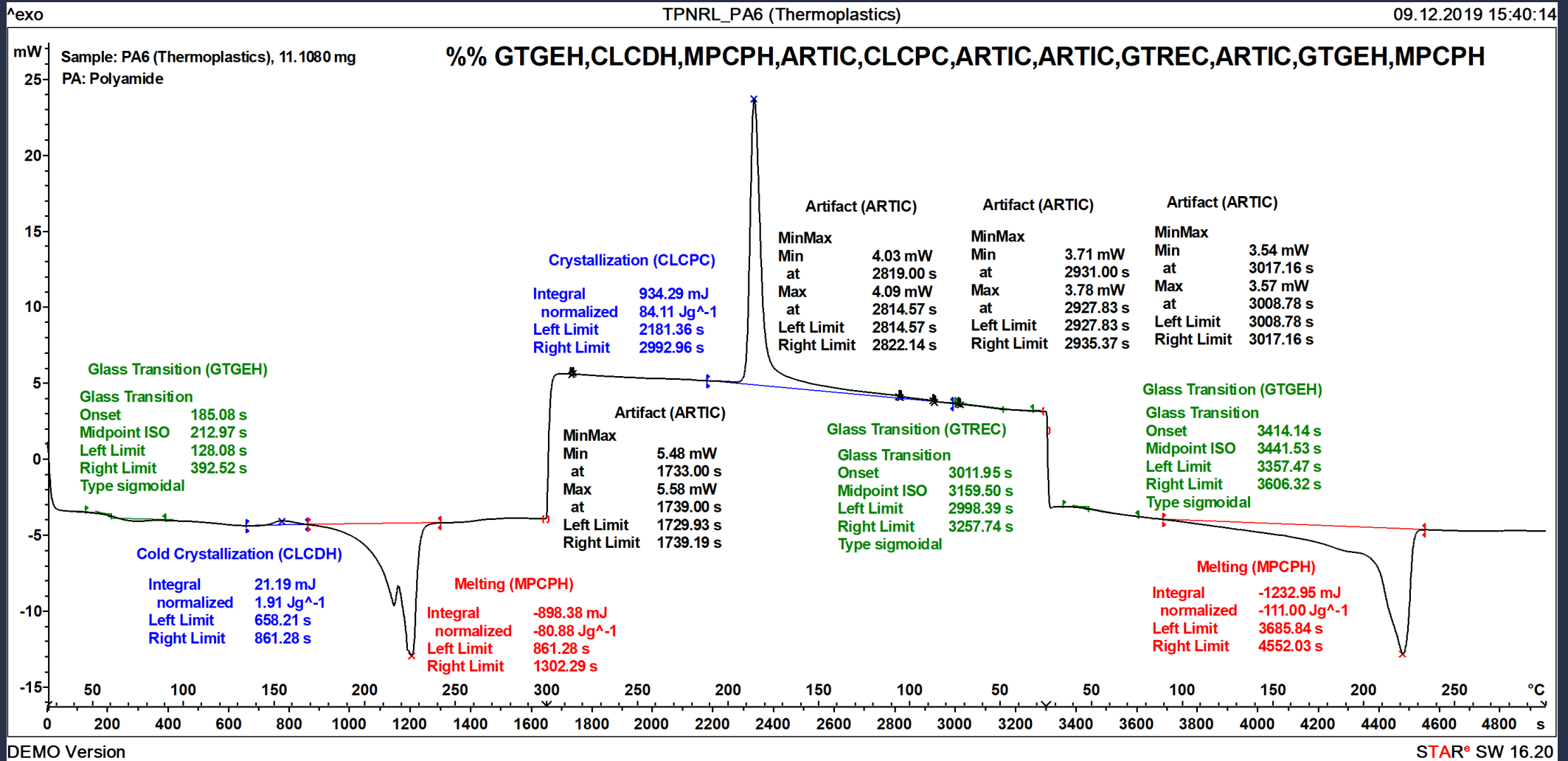
Today a manual,
time-consuming process



Honey with water



Complexity without limits



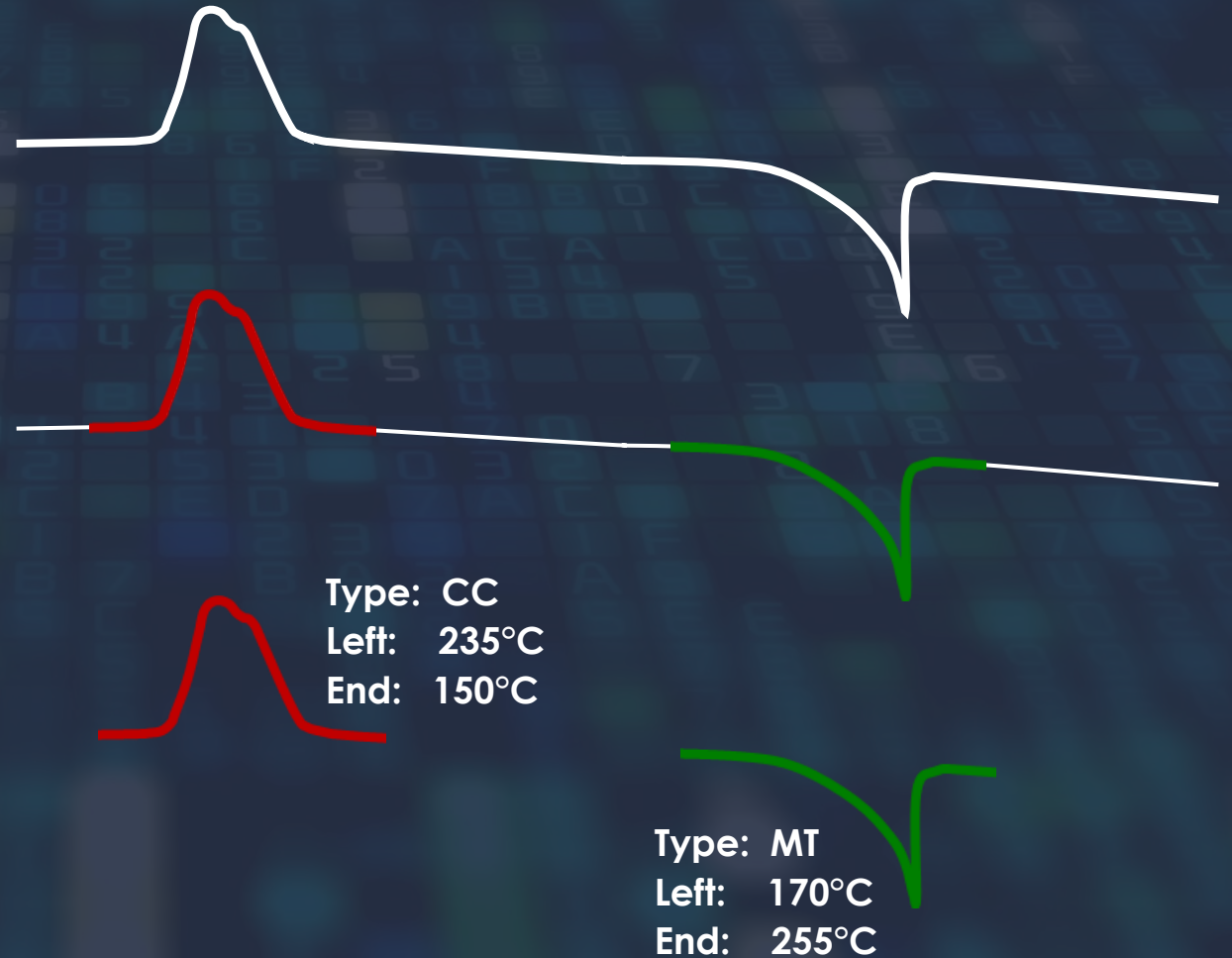
Algorithm Pipeline

Raw Signals

Segmentation

Separation

Classification



Rare Data

16 material groups

27 possible effect types

Data from devices up to 30 years old

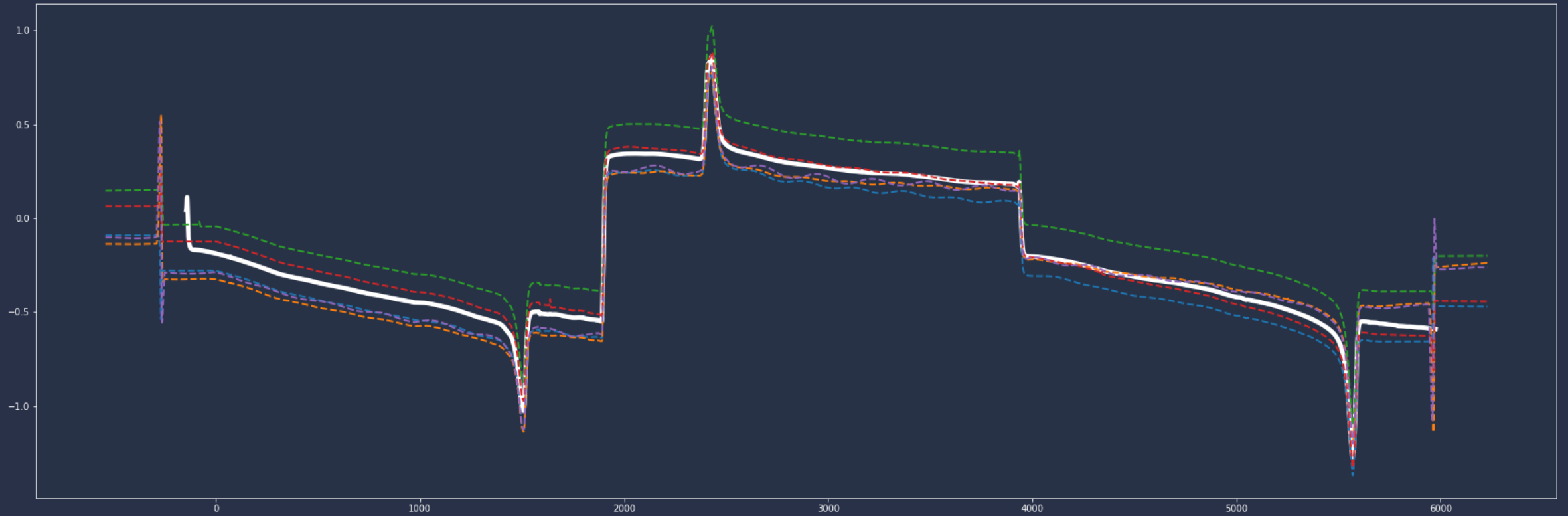
Different device usage



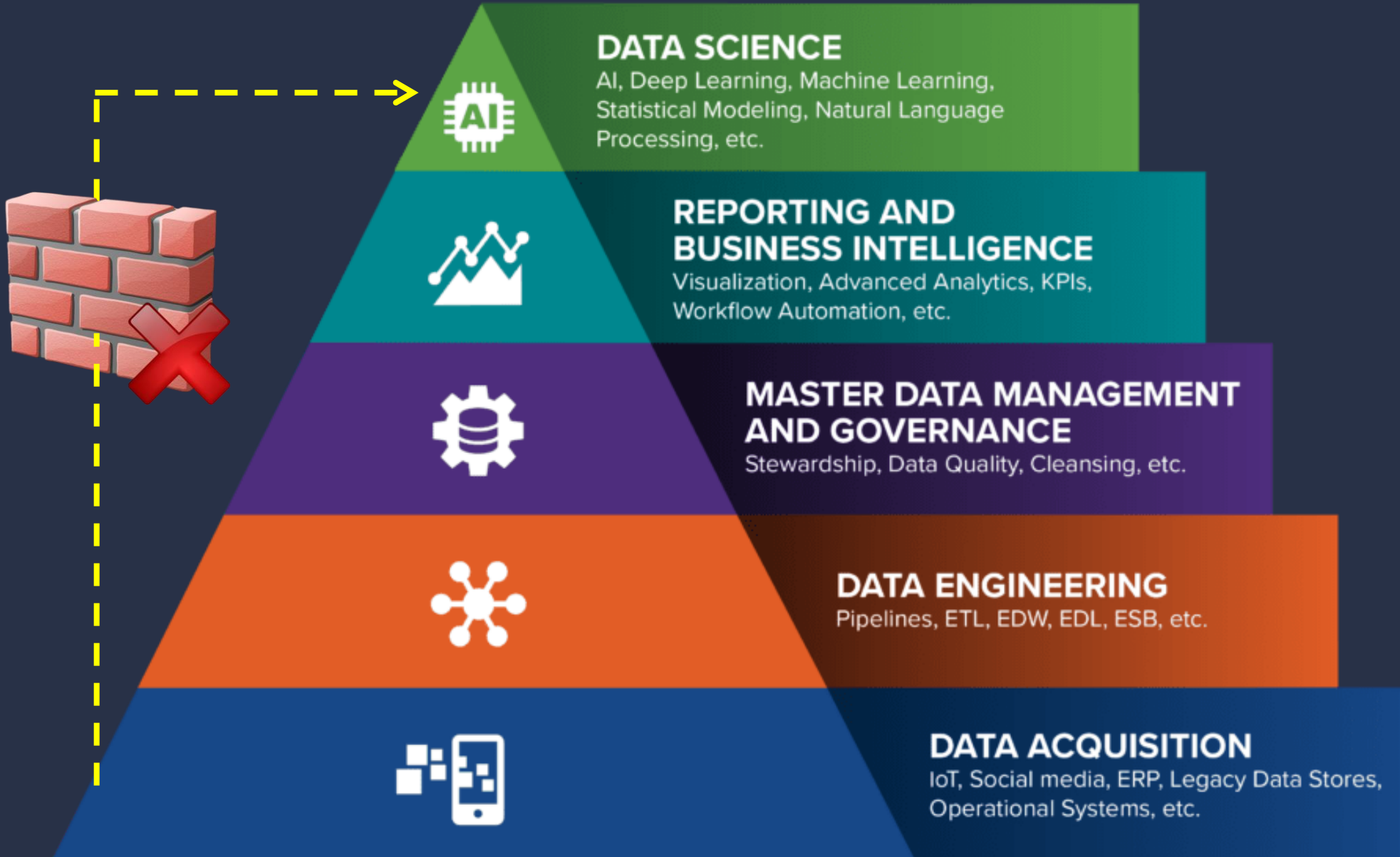
Too much variation for too little data!

Solution

- Variation Reduction
- Data Augmentation



The Data Science Pyramid



Expert Evaluation

- 109 Curves with AIWizard network:

Evaluation	Total	Perc.
Good	42	38.5 %
Medium	46	42.2 %
Bad	21	19.3 %

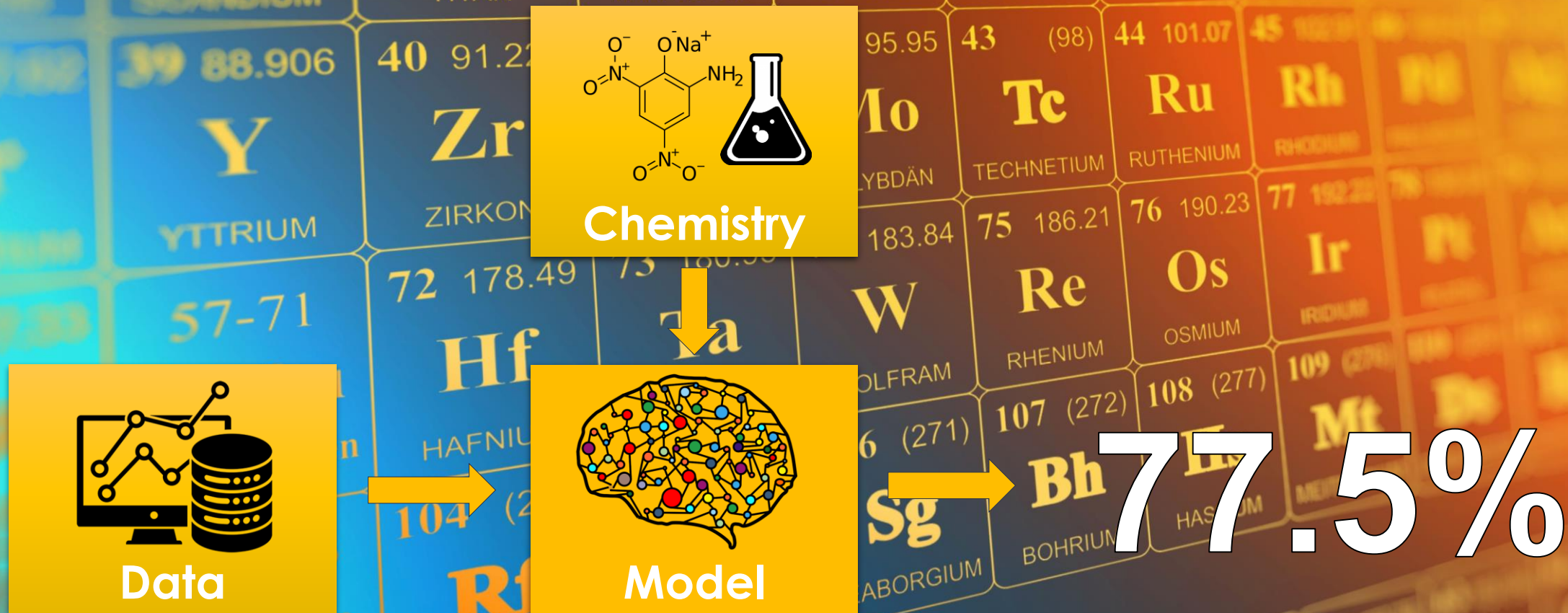
- Scenarios where algorithm fails:
 - Multiple detections for same effect
 - High dynamic curves
 - Artifacts arising from device get detected as effect

Solution ?

- Large number of machine-learning approaches tested
- Promising architectures, but always severe overfitting
- Not enough data to really learn chemical behavior



Chemistry-informed neural network



AI Knowledge? We Need Support!

- 17.8.2018 A possibility in UK? (No, their idea was not really AI based → ☹)
- 31.8.2018 From a former project I remembered Prof. Ch. Heitz
- Idea was distributed within this network
- 14 CH research teams drafted ideas
- 3 Teams selected to present idea live
- 28.10.2018 Decision
- Two teams with different but complementary approaches: ZHAW (Statistics) und CSEM (AI)
- Innosuisse (submitted 06.2019, approved 10.0229)
- Start project 12.2019 (24 + 5 months)



Innosuisse - Swiss Innovation Agency



Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra

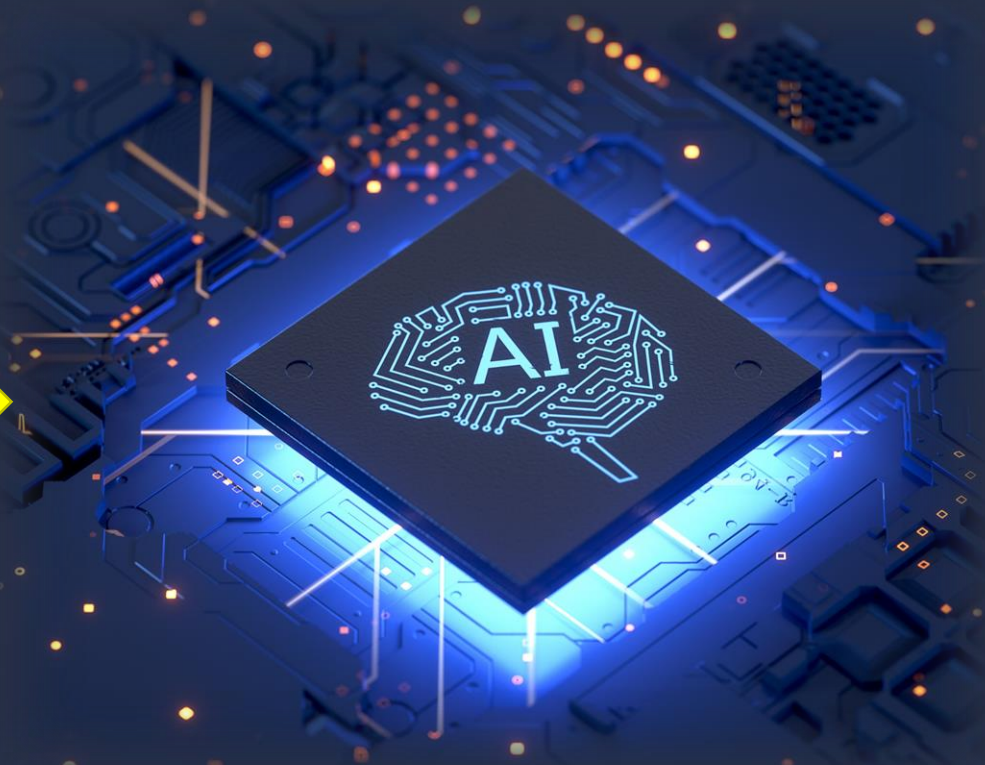
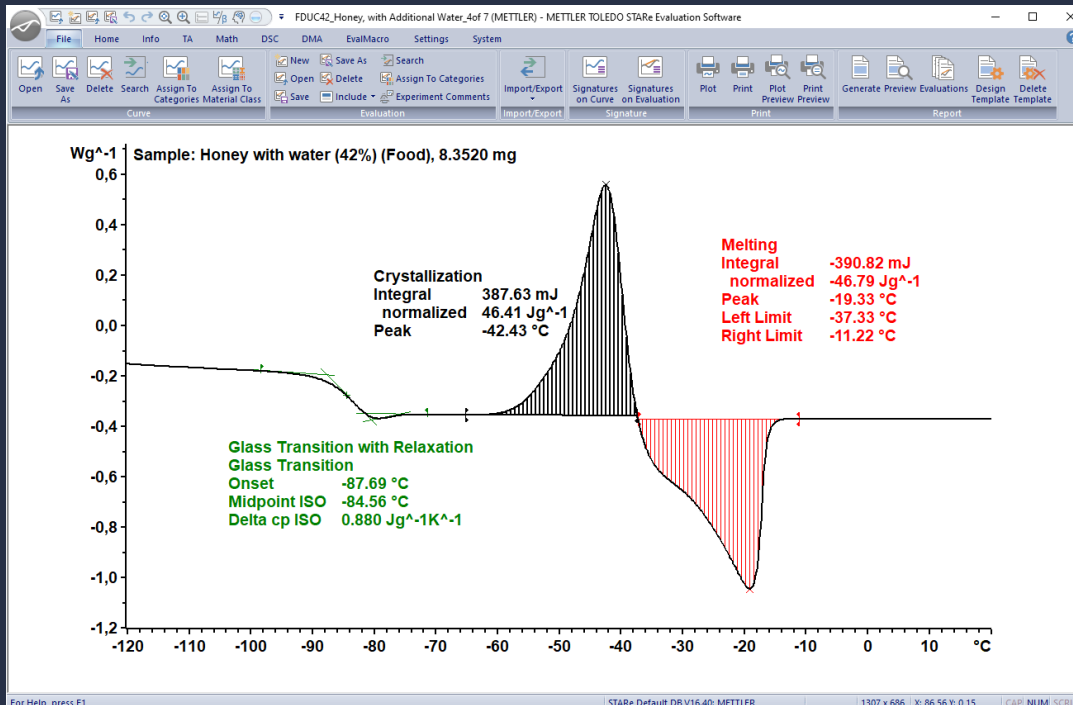
Project-Team

4 Teams → One Goal

- ZHAW (Statistics) 1
- CSEM (AI) 6
- MT (Data+Commercial) 14
 - PM/Marketing 3 (+1 ext Video)
 - Patent 1 (+1 extern)
- MT (R&D) 2

Integration

- AIWizard is integrated in MTs software suite *STAR^e*
- Challenging integration: *STAR^e* was released in 1992
- Inferencing < 1 sec modern laptop
- No GPU required



AI Integration – Obfuscation!

- Protect intellectual property
- Prevent an attacker from reverse engineering
- Obfuscation, compilation to binary, security



AIWizard.py

utils.py



AIWizard.pyd

utils.pyd

```
4 class Model():
5     def __init__(self, binary, config) -> None:
6
7         self.config = config
8         self.session = onnxruntime.InferenceSession(binary)
9
10        self.input_names = [x.name for x in self.session.get_inputs()]
11        self.output_name = self.session.get_outputs()[0].name
```

```
1  00000000 4d 5a 90 00 03 00 00 00 04 00 00 00 ff ff 00 00
2  00000100 b8 00 00 00 00 00 00 00 40 00 00 00 00 00 00 00
3  00000200 00 00 00 00 00 00 00 00 00 00 00 00 00 00 00 00
4  00000300 00 00 00 00 00 00 00 00 00 00 00 00 08 01 00 00
5  00000400 0e 1f ba 0e 00 b4 09 cd 21 b8 01 4c cd 21 54 68
6  00000500 69 73 20 70 72 6f 67 72 61 6d 20 63 61 6e 6e 6f
```

Market Introduction

Sales & service training April 2022

Customers are very interested and provide new data for future neural network improvements

AIWizard is a sellable options of the STAR^e Software offering

First paying customer orders received 😊

∴ csem METTLER TOLEDO

The screenshot shows the Mettler Toledo website page for AIWizard. The header includes the Mettler Toledo logo and navigation links for Products & Solutions, Industries, Services & Support, Events & Expertise, About Us, and Contact Us. The main content area features a 'Know How' section with the title 'AIWizard – Artificial Intelligence for Thermal Analysis' and the subtitle 'Enhance Your Laboratory's Automation Capabilities'. The text describes AIWizard as a revolutionary AI solution for thermal analysis result evaluation and thermal event identification. It highlights that AIWizard is trained on thousands of expert evaluation examples and can adapt and learn beyond model limitations. A 'Download Information Sheet' button is prominently displayed. Below it, there is a link to 'Learn about the AIWizard in our short video.' At the bottom, there is a section for 'AIWizard Neural Network Download' with instructions to follow a link to download the neural network for the user's STAR^e software version, noting that the prerequisite is the AIWizard option in the STAR^e software. A link for 'AIWizard Neural Network Download' is provided.

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Knowledge and Expertise Resources > AIWizard – Artificial Intelligence for Thermal Analysis

Know How

AIWizard – Artificial Intelligence for Thermal Analysis

Enhance Your Laboratory's Automation Capabilities

AIWizard™ is a revolutionary artificial intelligence (AI) solution for thermal analysis result evaluation and thermal event identification.

Using a trained neural network built into the STAR^e software, the AIWizard autonomously identifies and evaluates all thermal effects measured by DSC. This intelligent neural network, which was trained using thousands of expert evaluation examples, can adapt and learn beyond the limitations of a model, enabling the AIWizard to accurately detect all thermal effects.

Enable your methods with AIWizard to enhance your laboratory's automation capabilities. Set up experiments that are automatically evaluated, freeing up time for your analysts so they can focus on sample preparation and drawing the right conclusions from the evaluation.

Download our free information sheet to discover more about AIWizard.

[Download Information Sheet](#)

▶ [Learn about the AIWizard in our short video.](#)

AIWizard Neural Network Download

Follow the link below and go to the AIWizard™ tab to download the relevant neural network for your STAR^e software version.

Prerequisite: AIWizard option in the STAR^e software.

▶ [AIWizard Neural Network Download](#)

The thumbnail image shows the cover of the 'AIWizard - Autonomous Processing of Thermal Analysis Measurements' information sheet. It features the Mettler Toledo logo and a graphic of a circuit board.

Perspectives

Time is critical, usage of expert knowledge makes often sense!

To combine the expert knowledge from academia and/or engineering companies can speed up the introduction of exciting new products.

Key take aways

- The business idea must be the starting point
- Industry as the project driver is a given
- A functional model is not a commercial product
- Close cooperation is important (full engagement of all employees)
- Parallel development (technology and commercial product project) is a risk, but it reduces the overall project time

Our conclusion

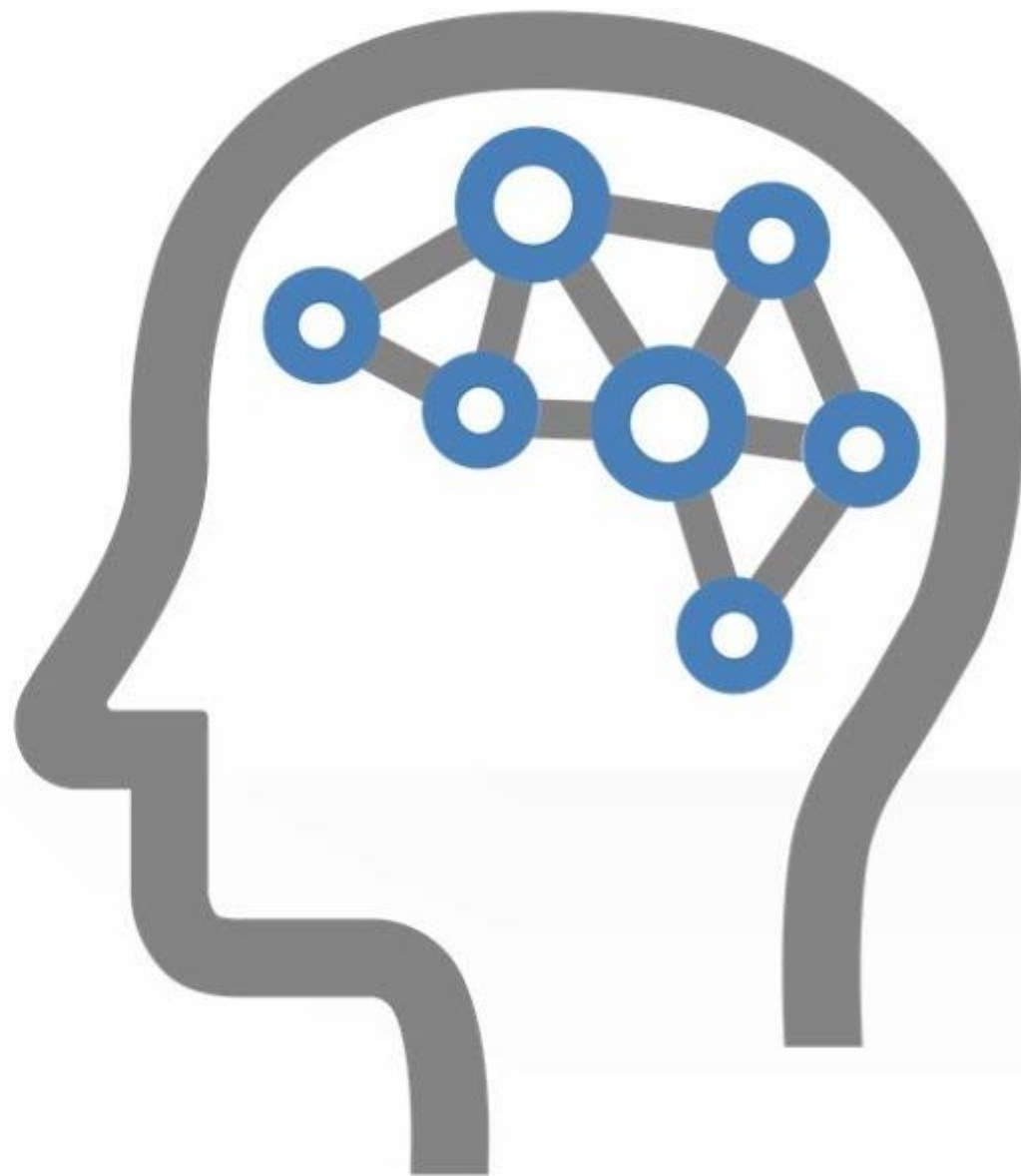
- A win-win situation → new projects have already started ...



AIWizard™

Autonomously identifies
and evaluates all types
of thermal effects

[Link Video](#)



METTLER TOLEDO

Laboratory Solutions



csenm

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