

STK, September, 2025
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AIWizard™

Intelligent and automatic DSC curve evaluation

'Credits shall be given to Authors for any use of this materials !'

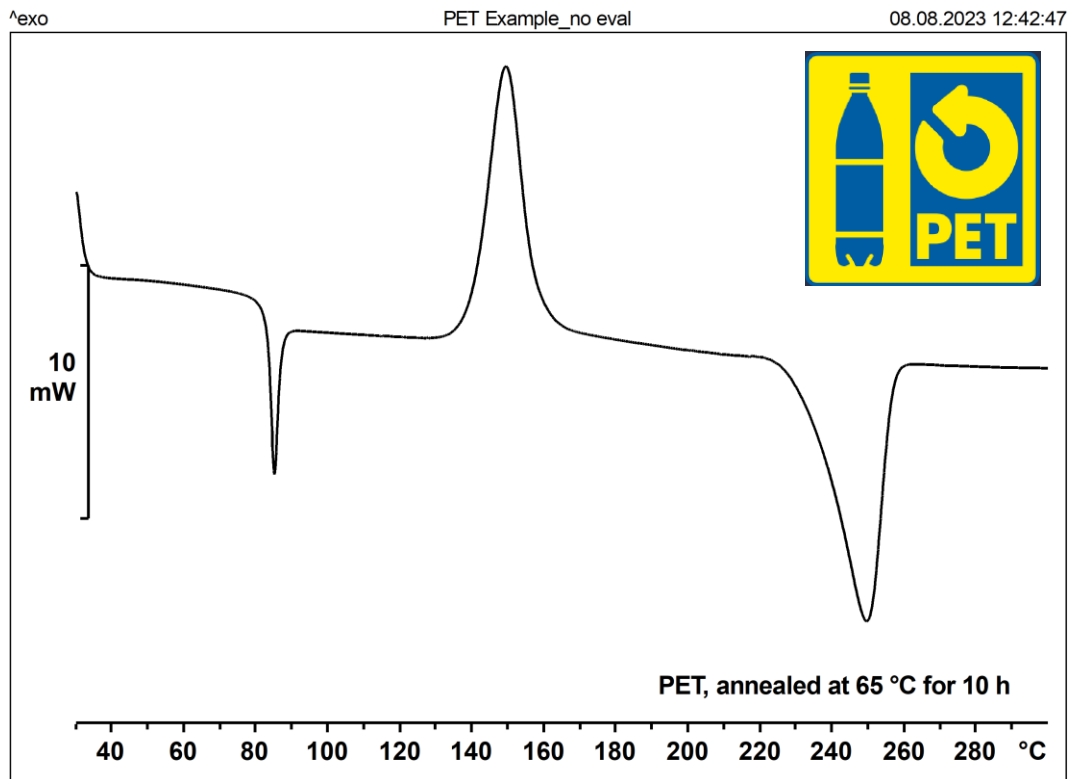
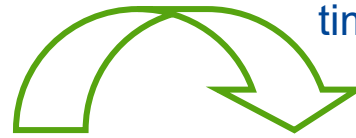
METTLER TOLEDO

The logo graphic for Mettler Toledo, featuring a stylized green and blue arrow pointing upwards and to the right, composed of multiple parallel lines.

Evaluating thermal analysis measurements leaves many analysts questioning:

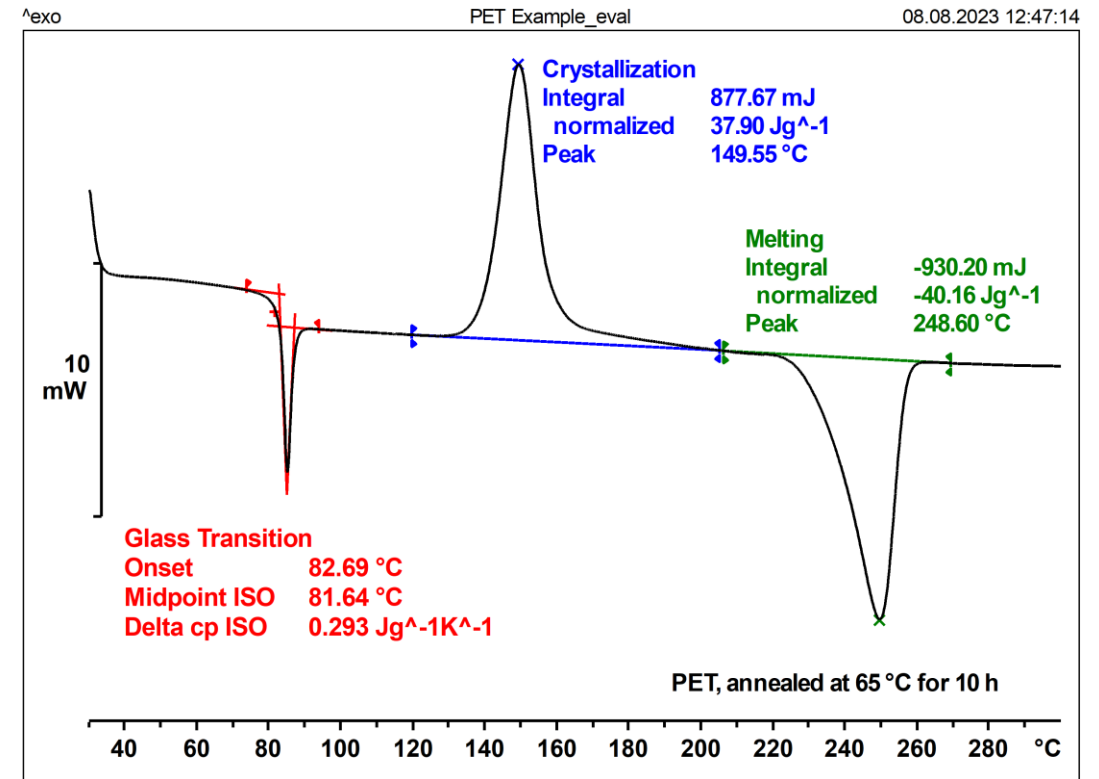
- Effect or artifact?
- What effect is it?
- Begin and end of effect?

Today a manual,
time-consuming process



DEMO Version

STAR® SW 18.00



DEMO Version

STAR® SW 18.00

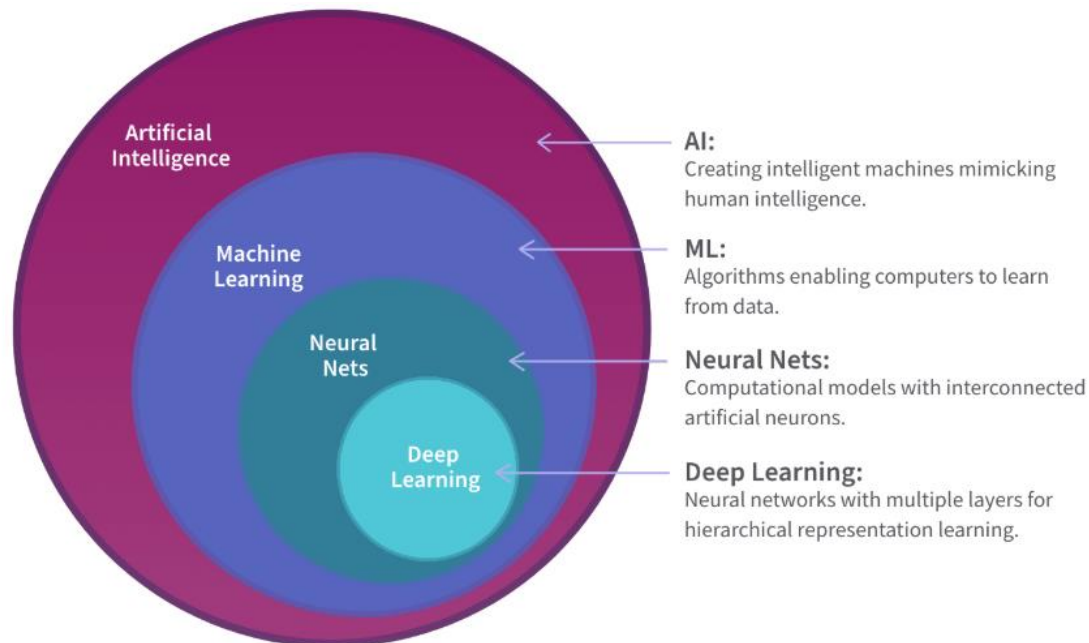
Artificial Intelligence vs. Mathematics

- **Mathematical approaches** rely on algorithms and models. Therefore, the results are only as good as how well the real-life situation is simulated. In some cases models may work, but in others they fail.
- **Artificial intelligence** instead uses neural networks, which can adapt and learn beyond the limitations of a model.
- This enables the AIWizard™ to accurately detect all thermal effects.

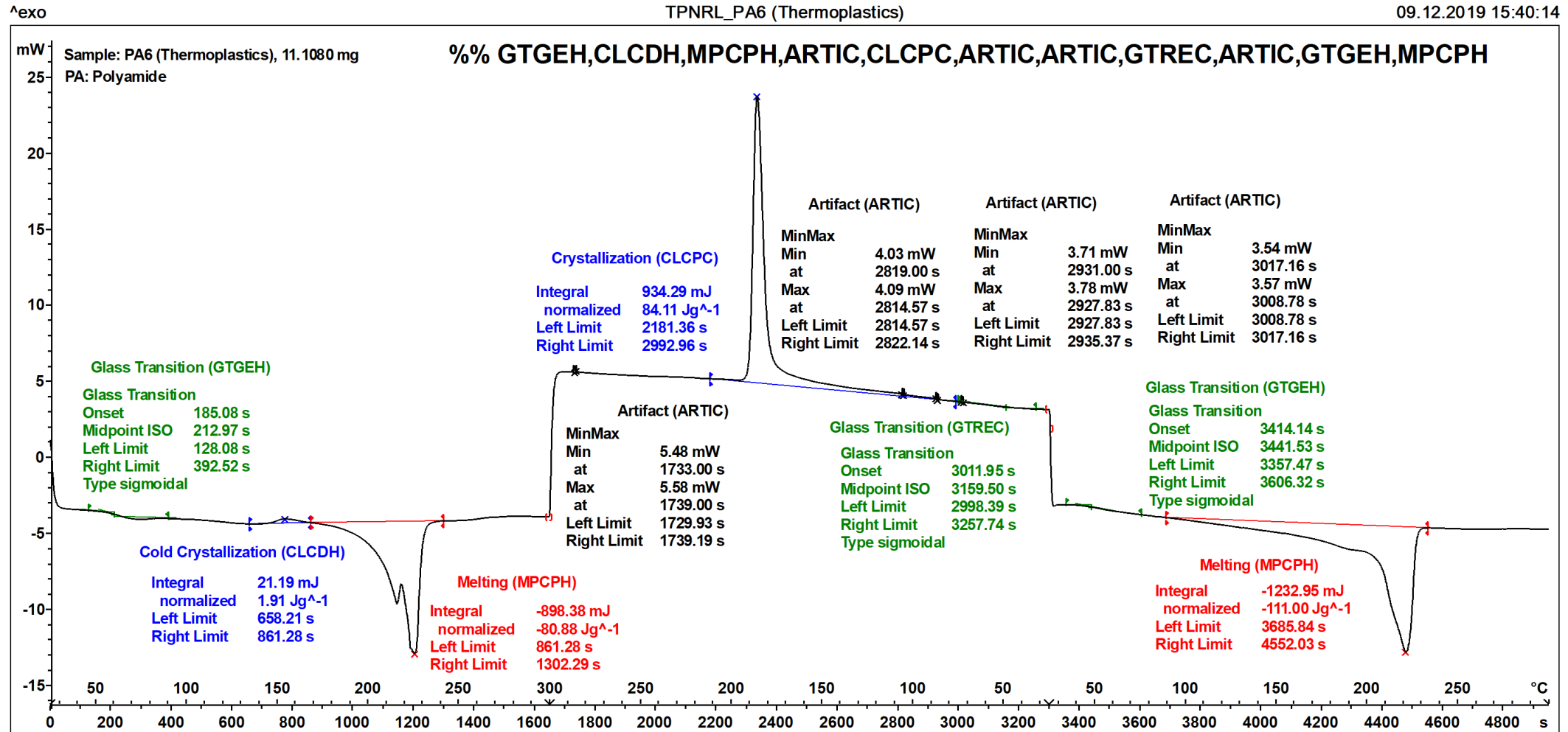


ML is a specific subset of AI focused on enabling machines to learn from data

- **ML** can be defined as the process of developing algorithms and statistical models that are then used to analyze data and recognize patterns.
- **AI** is essentially the byproduct of ML and is more concerned with the creation of computer systems and technologies that can then be programmed with machine learning algorithms.
- **Neural networks** are a specific type of machine learning model, inspired by the structure of the human brain and are a tool within the larger toolkit of machine learning techniques.

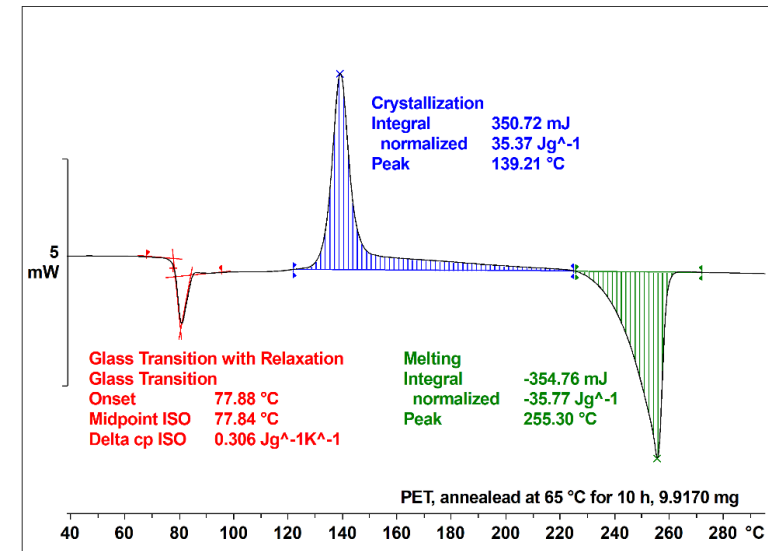
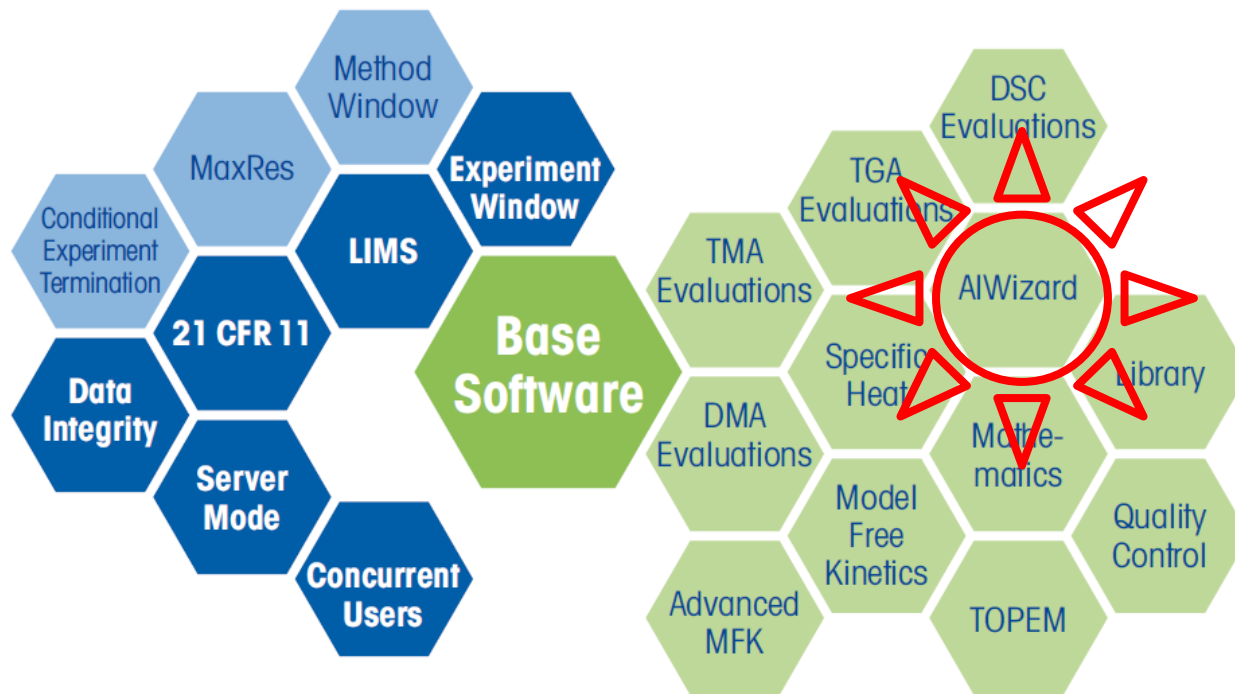


Data preparation and review



New STAR^e software option released in 2022

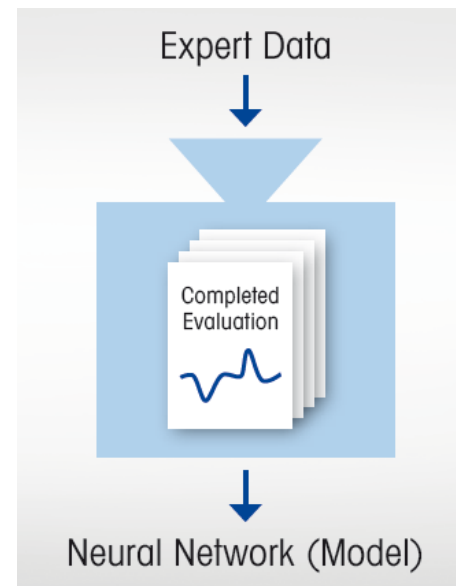
Productivity increase and higher result quality thanks to a fully automatic evaluation and interpretation of an unknown material measured by DSC



Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra
Swiss Confederation
Innosuisse – Swiss Innovation Agency

Functionality and capabilities

- **Neural networks** are the core of artificial intelligence and are trained with expert data. The resulting system is used to analyze a new set of data.
- For the **AIWizard™**, we are using a **commercial AI algorithm** in combination with data processing.
- We can take into account the **material class** if one is selected for the curve.
- We have reviewed thousands of evaluations (expert data) so that they could be used to train the neural network.

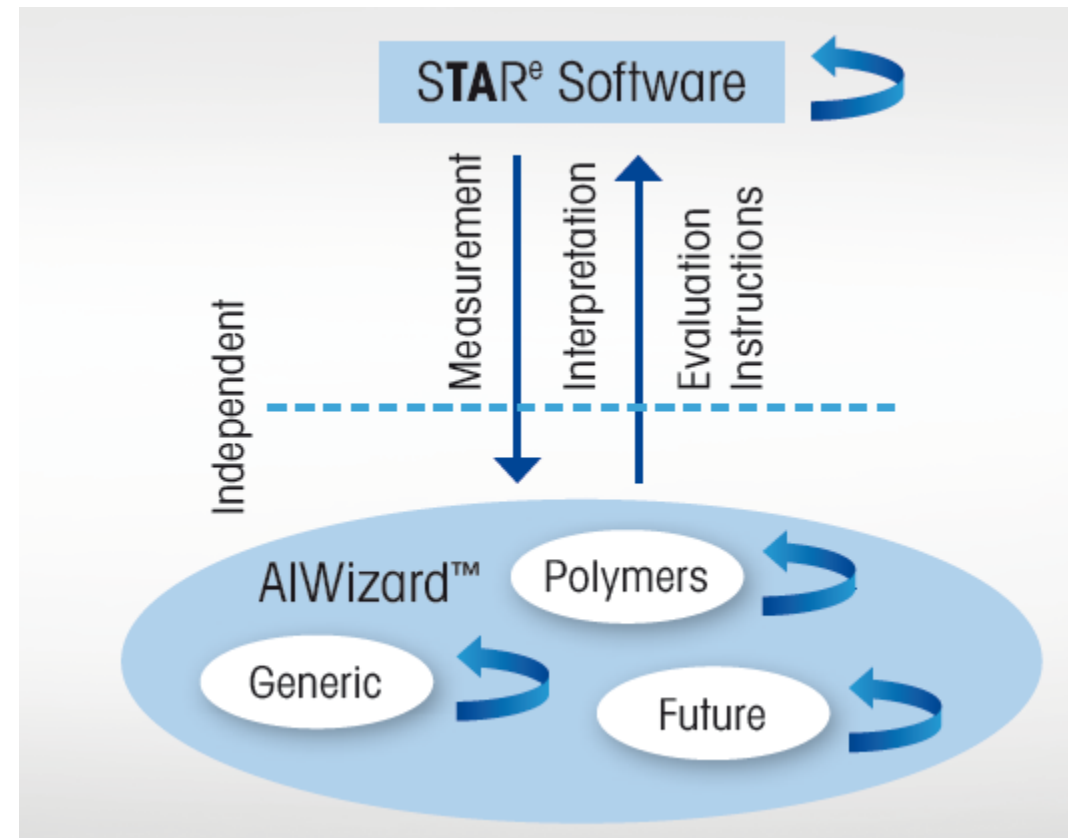


Two models:

1. DSC Polymers V2
2. DSC Generic V2

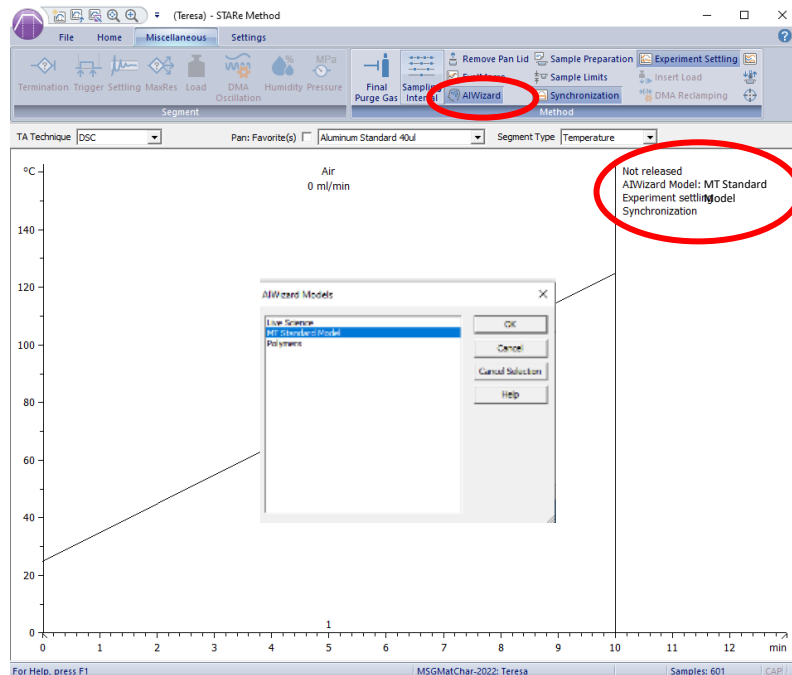
Model store – easy update without STAR^e SW changes

- Challenging integration: STAR^e was released in 1993
- Capability to have multiple neural networks
- The AIWizard™ is based on a database (model store) containing one or more neural networks
- Measurement data is sent from STAR^e to the AIWizard™ where it is interpreted. The interpretation is then sent back to STAR^e.
- This clever design allows either networks or the STAR^e software to be updated independently.



Updates will be released whenever more data is available for training a specific neural network or to enhance the generic network.

Autonomous analysis and interpretation

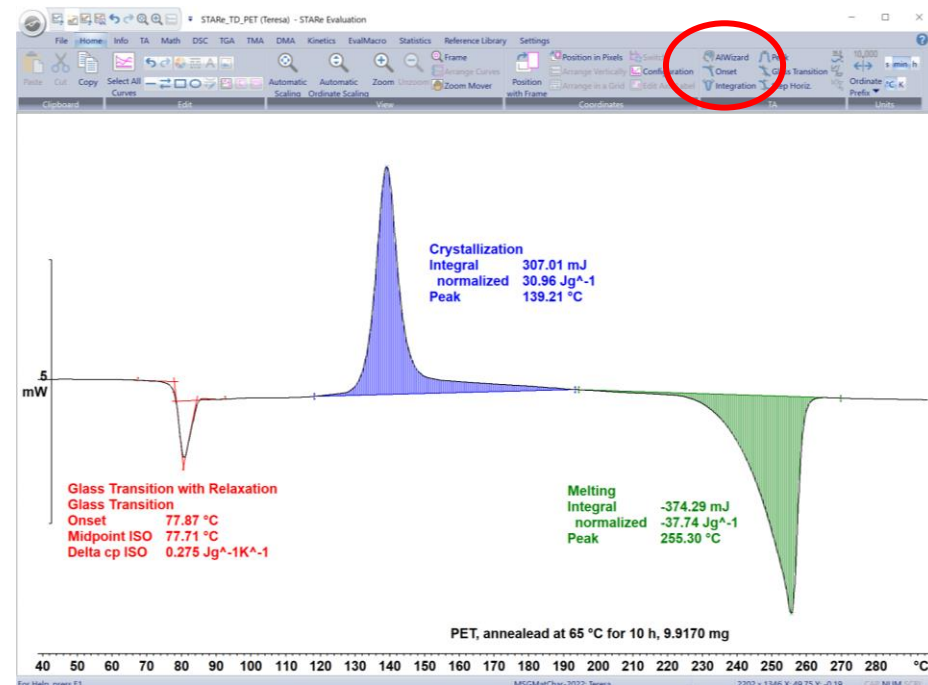


- In the Method window, the AIWizard™ can be activated. This enables automatic identification and evaluation at the end of the experiment.
- Free up time for analysts so they can focus on sample preparation and drawing the right conclusions from the evaluation.

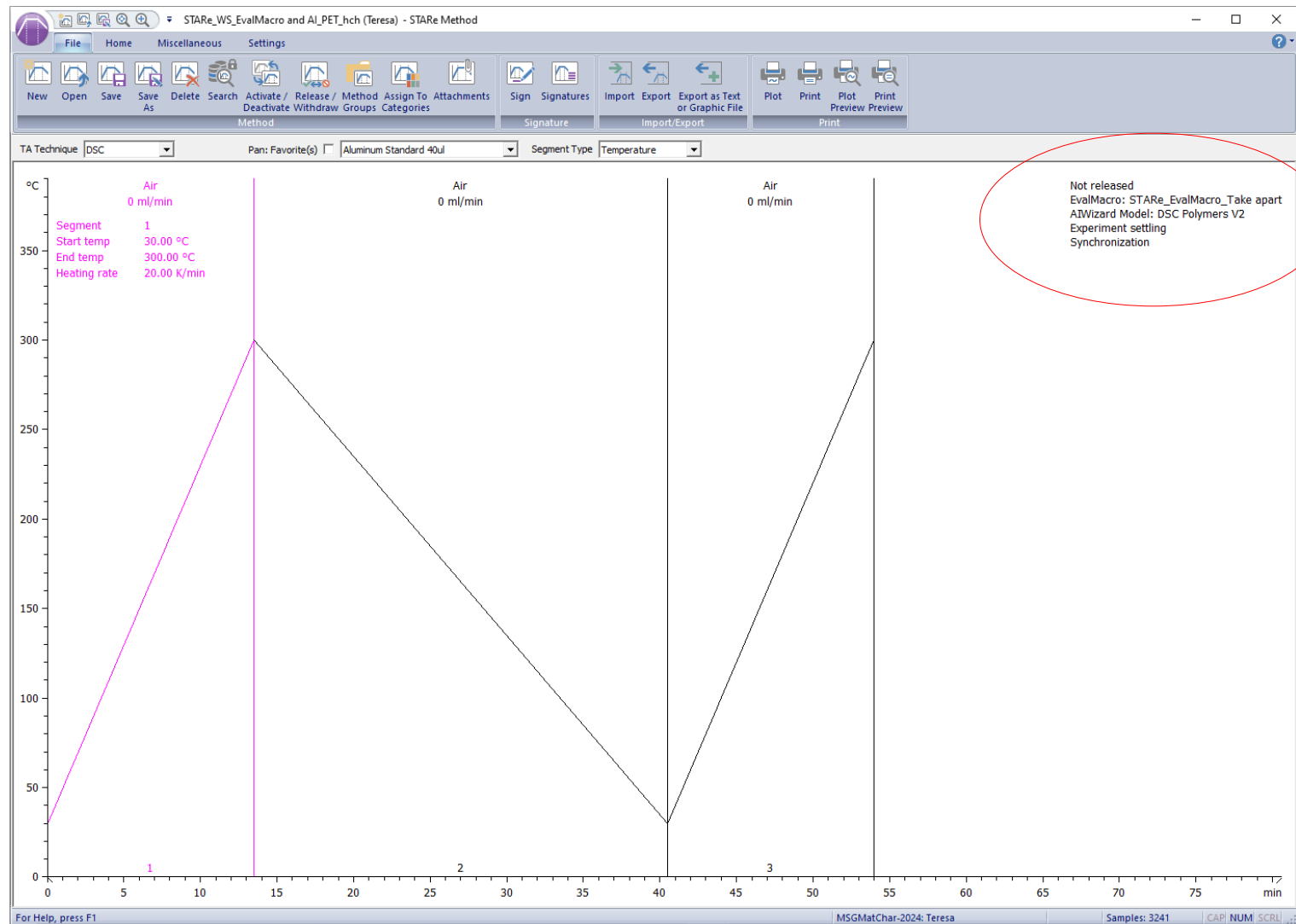
AIWizard™ as a second opinion



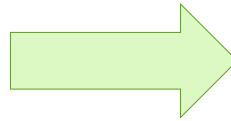
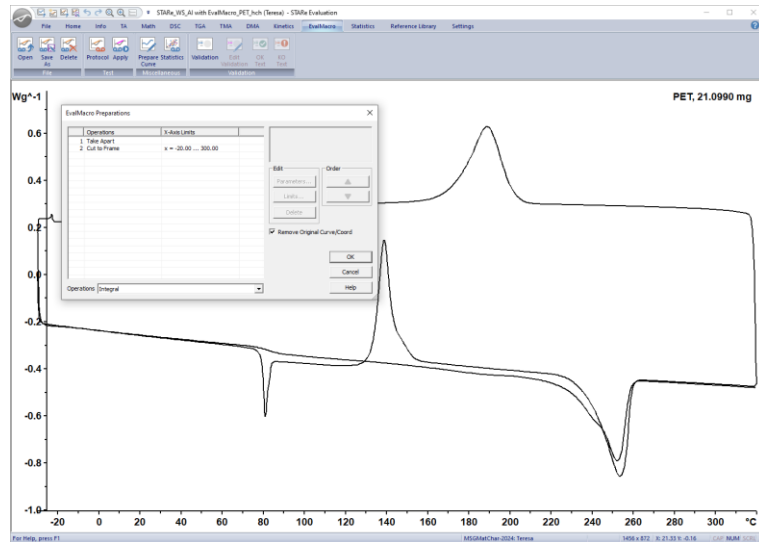
- The manual evaluation feature allows users to select the AIWizard™ in the evaluation window and to reduce evaluation time.
- Using the AIWizard™ manually offers:
 - A second expert opinion or
 - A fast one click evaluation possibility



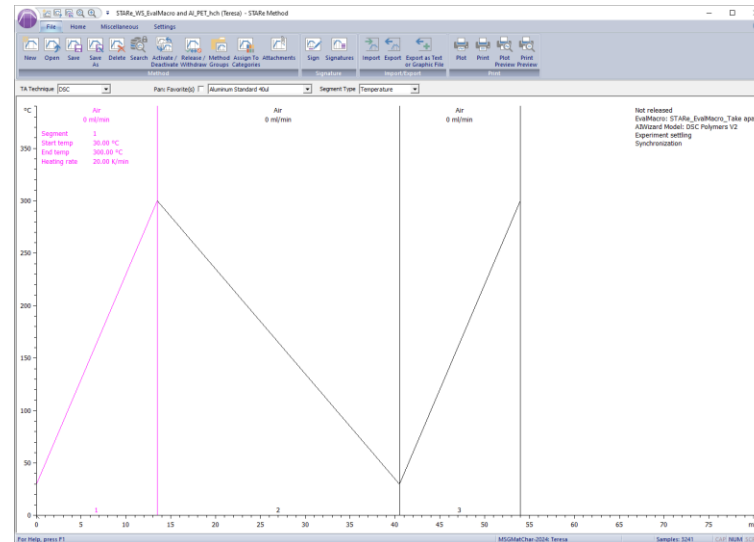
Both Eval Macro and AIWizard automatic evaluation can be attached to the method



1. Prepare curve with EvalMacro

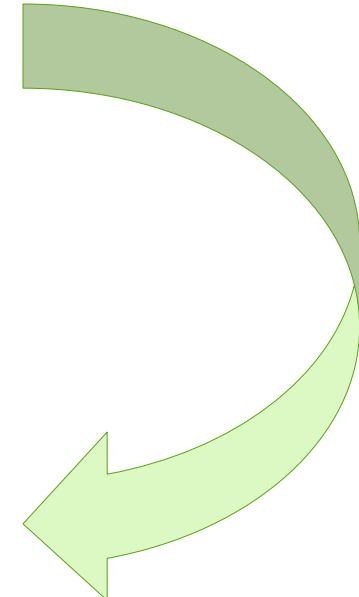
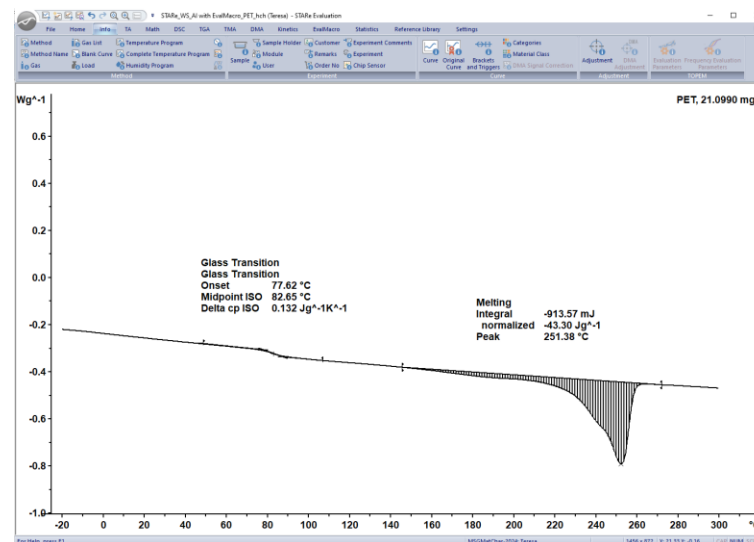


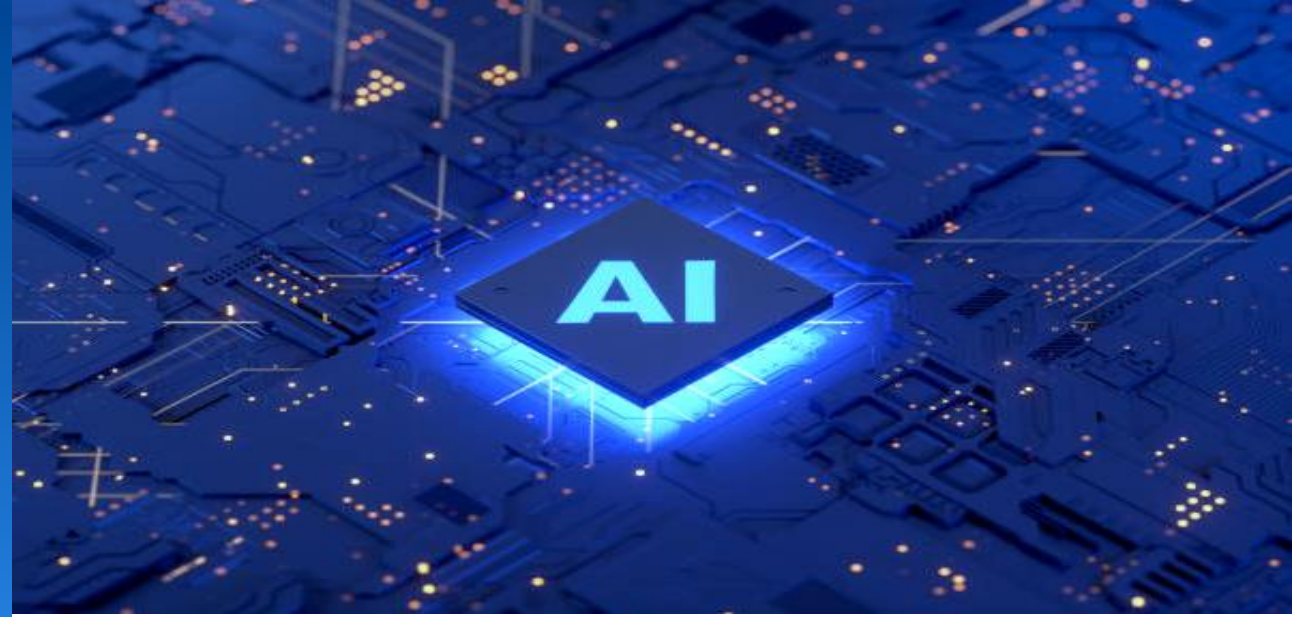
2. Create method with EvalMacro and AIWizard



- Prepare curve with EvalMacro
- Automatic evaluation with AIWizard

3. Get evaluation





Thank you

Cooperation Partners



Much variation for little data

- 19 different material classes
- More than 25 possible effect types
- More than 2500 DSC curves (for V1)
- More than 4200 effects labelled (for V1)
- Data from devices up to 30 years old
- Different device usage




More than 4100 hours for expert data review (for V1)!

- (Additional 1110 DSC curves for V2)

Overview for V1

Material	# DSC curves	# labelled events
Thermoplastics	666	1464
Thermosets	444	754
Elastomers	238	721
Organics	228	318
Food	170	248
Pharmaceuticals	150	218
PCM	80	83
Inorganics	77	116
Petrochemicals	55	92
Unknown	53	83
Metals	53	74
Biopolymers	23	59
Composites	6	9
Cosmetics	5	12
Energetics	1	3
Ceramic	1	2

The 4 stages of an experiment

Sample preparation	Measurement	Evaluation	Interpretation
	<p>Design of Cooling Segment</p> <p>Polymer blend, 16.2800 mg</p>	<p>Heating - Cooling - Heating Runs of PET</p> <p>PET: 10.2120 mg, heating rate: 20 K/min, cooling rate: 20 K/min</p> <p>First heating run Integral 308.71 mJ normalized 30.23 Jg⁻¹ Glass Transition Onset 79.02 °C Midpoint 79.18 °C Integral -364.45 mJ normalized -35.69 Jg⁻¹</p> <p>Cooling run Integral 403.55 mJ normalized 39.52 Jg⁻¹</p> <p>Second heating run Glass Transition Onset 83.91 °C Midpoint 92.08 °C Integral -405.89 mJ normalized -39.75 Jg⁻¹</p>	
	<p>Robot</p>	<p>EvalMacro</p>	<p>AIWizard</p>