Have Fun with AI Before We Begin!

Quick, Draw!

Blob Opera

Say What You See

Emoji Scavenger Hunt

Atoms and Algorithms

Exploring Artificial Intelligence for Chemistry

Sarah Clapham
Peter Hotchkiss
Office of Strategy and Policy

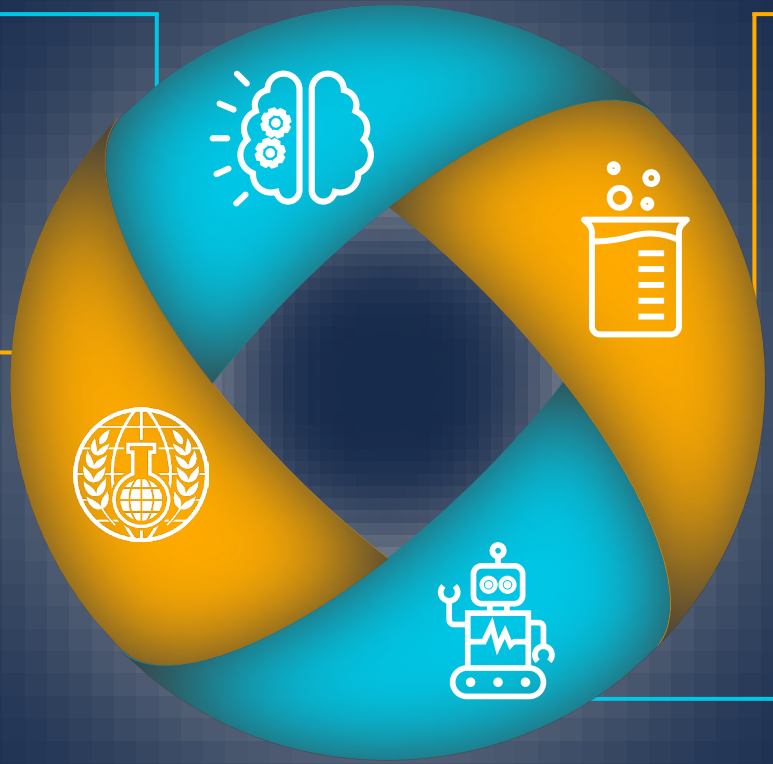
Günter Povoden
Scientific Advisory Board

OPCW
Organisation for the Prohibition of Chemical Weapons

AGENDA

01
Introduction to AI

02
AI in chemistry

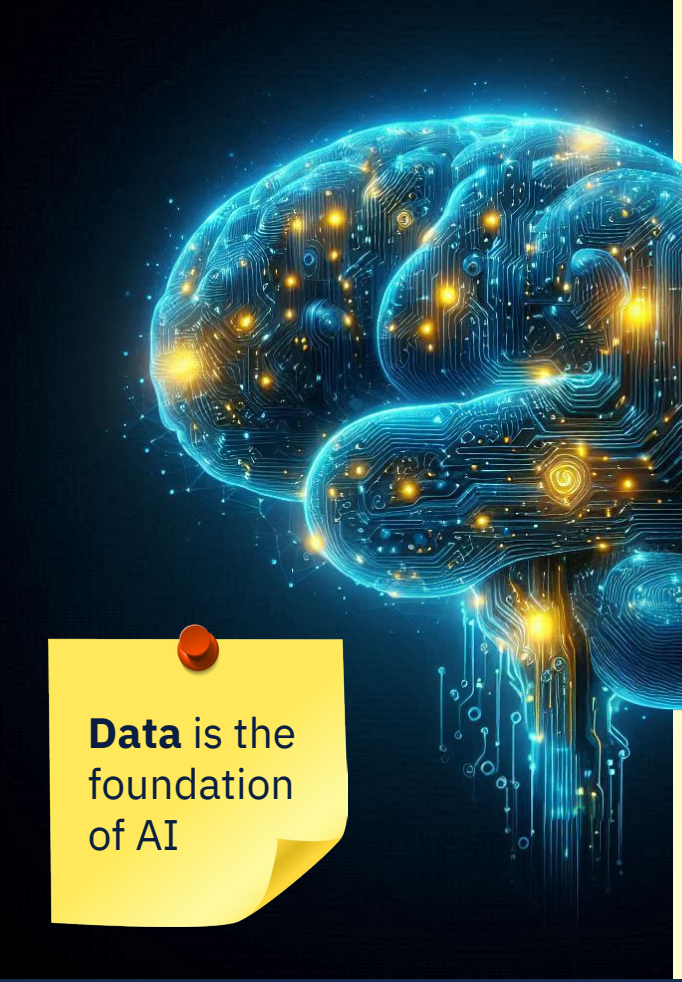


04
AI and the OPCW

03
Skills test

01

Introduction to AI



Data is the foundation of AI

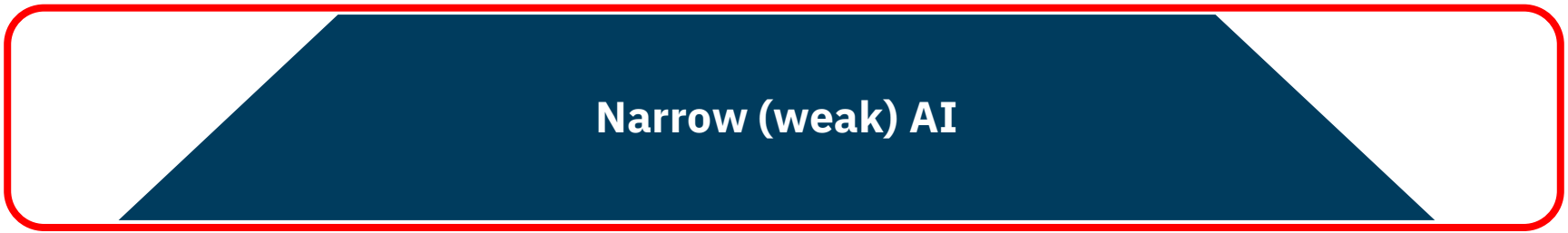
Artificial Intelligence (AI)

Machines or systems that mimic human intelligence

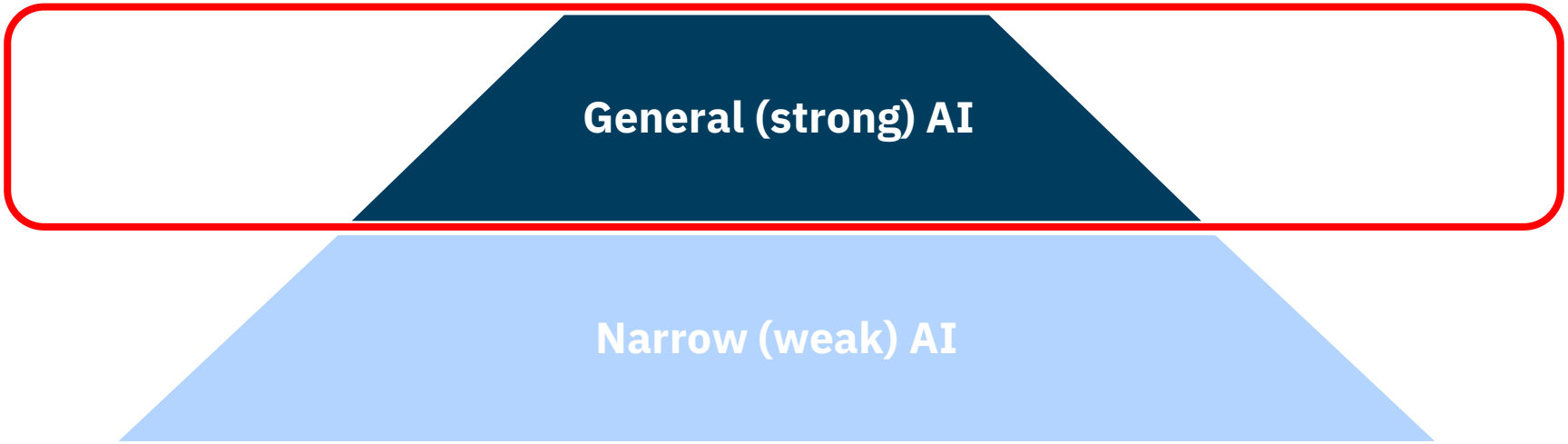
- Visual perception
- Speech recognition
- Problem solving
- Decision making

1956 – term first used

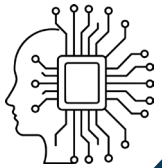
Categories of AI



Categories of AI



Categories of AI

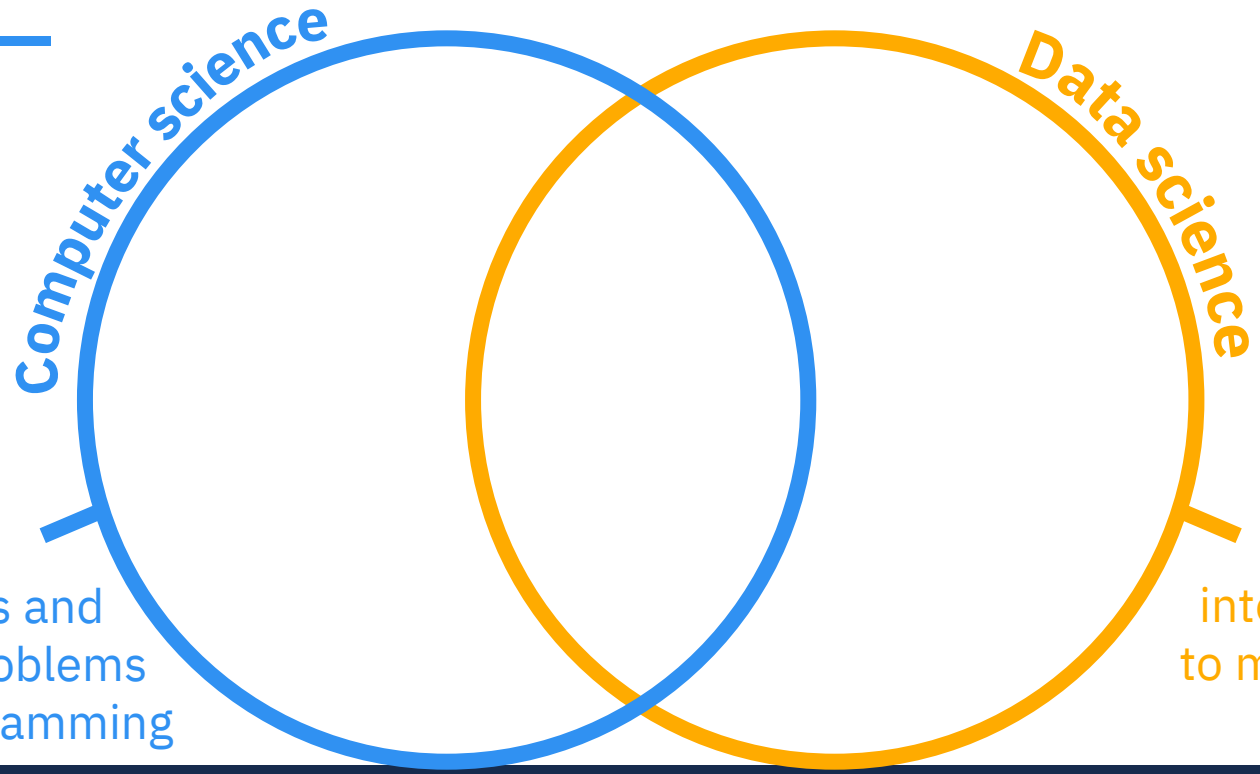


Super AI

General (strong) AI

Narrow (weak) AI

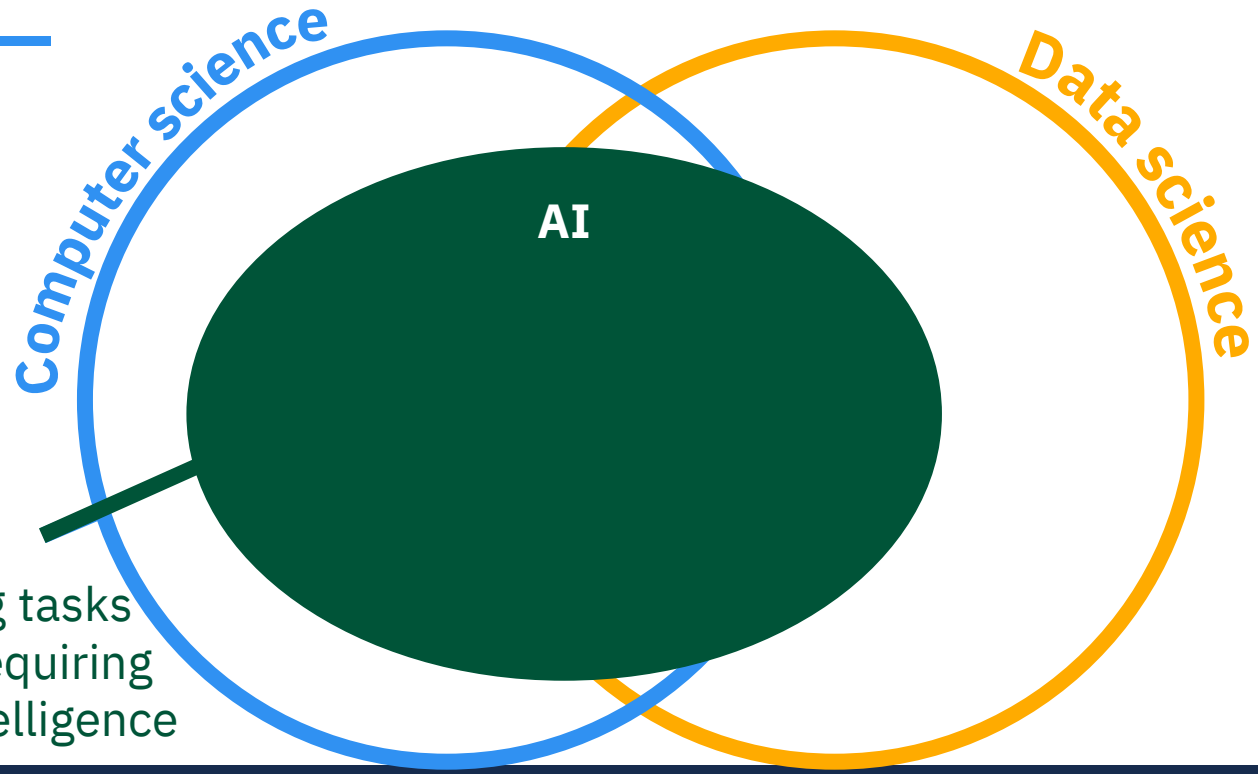
AI Ecosystem



Studying computers and solving problems with programming

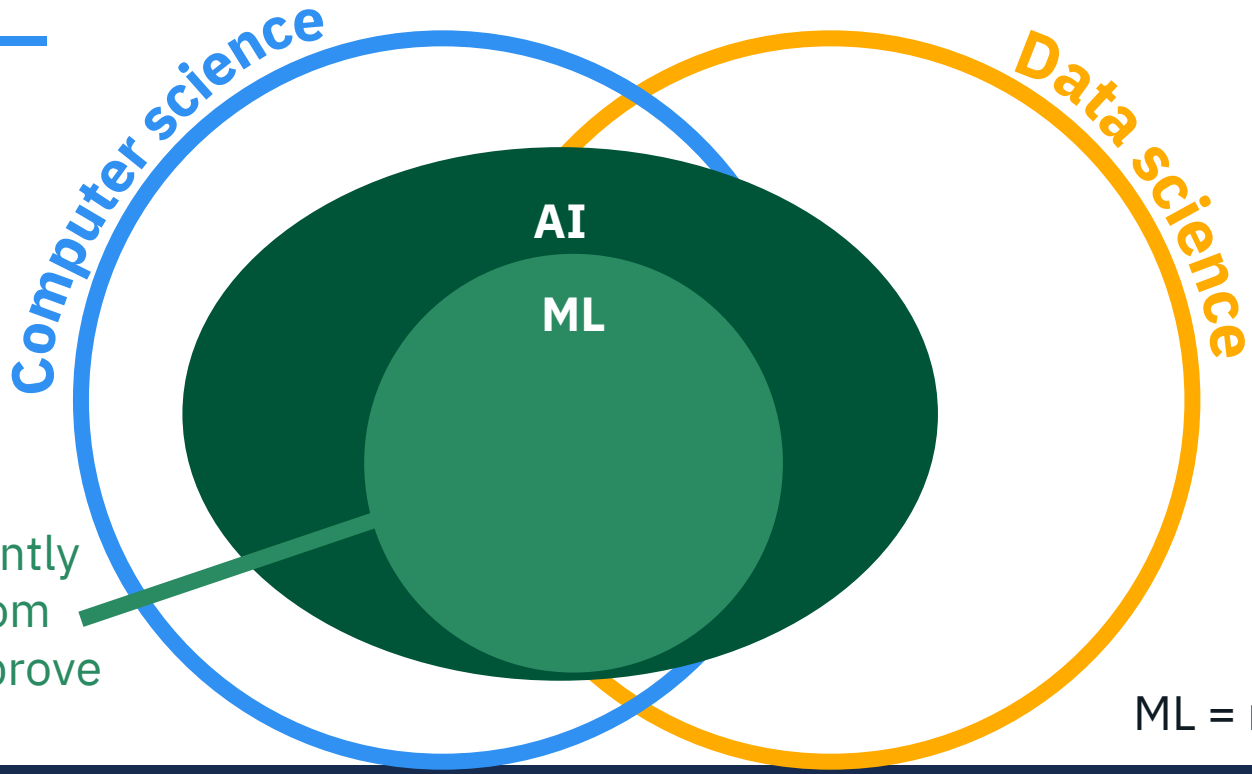
Analysing and interpreting data to make informed decisions

AI Ecosystem



Systems performing tasks typically requiring human intelligence

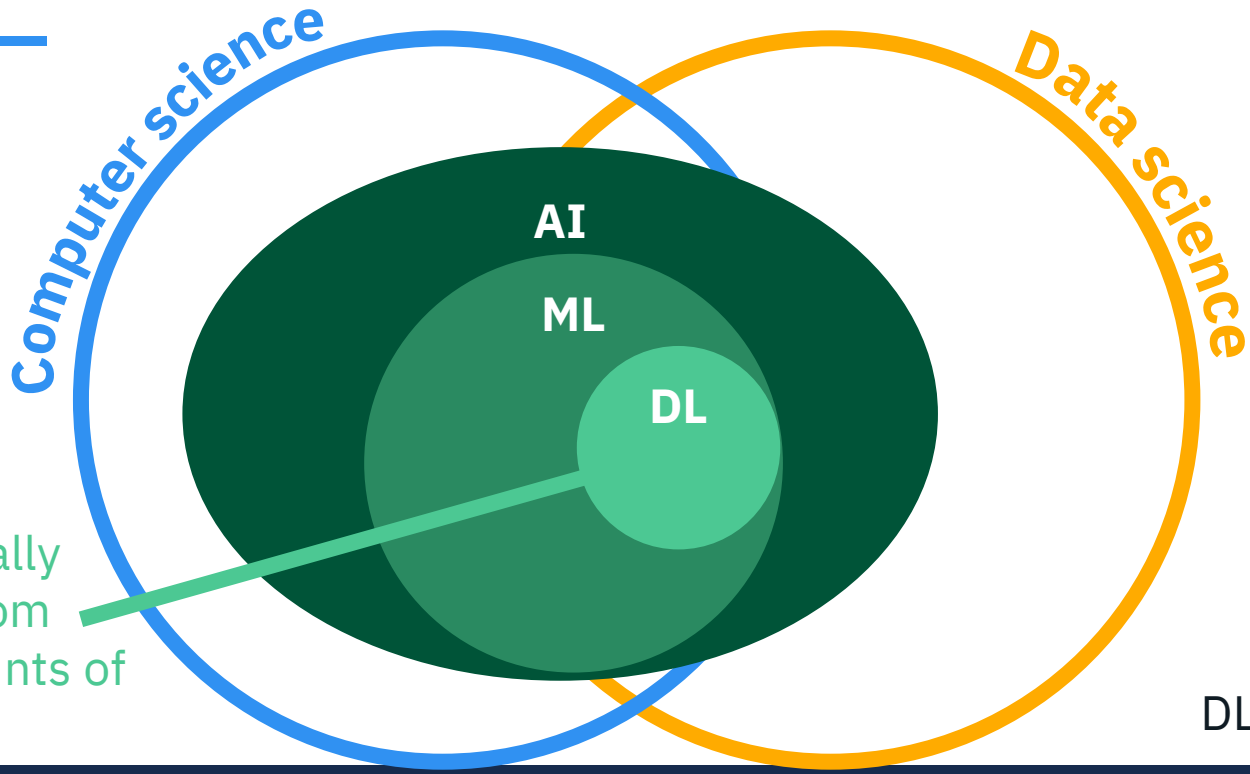
AI Ecosystem



Independently learning from data to improve over time

ML = machine learning

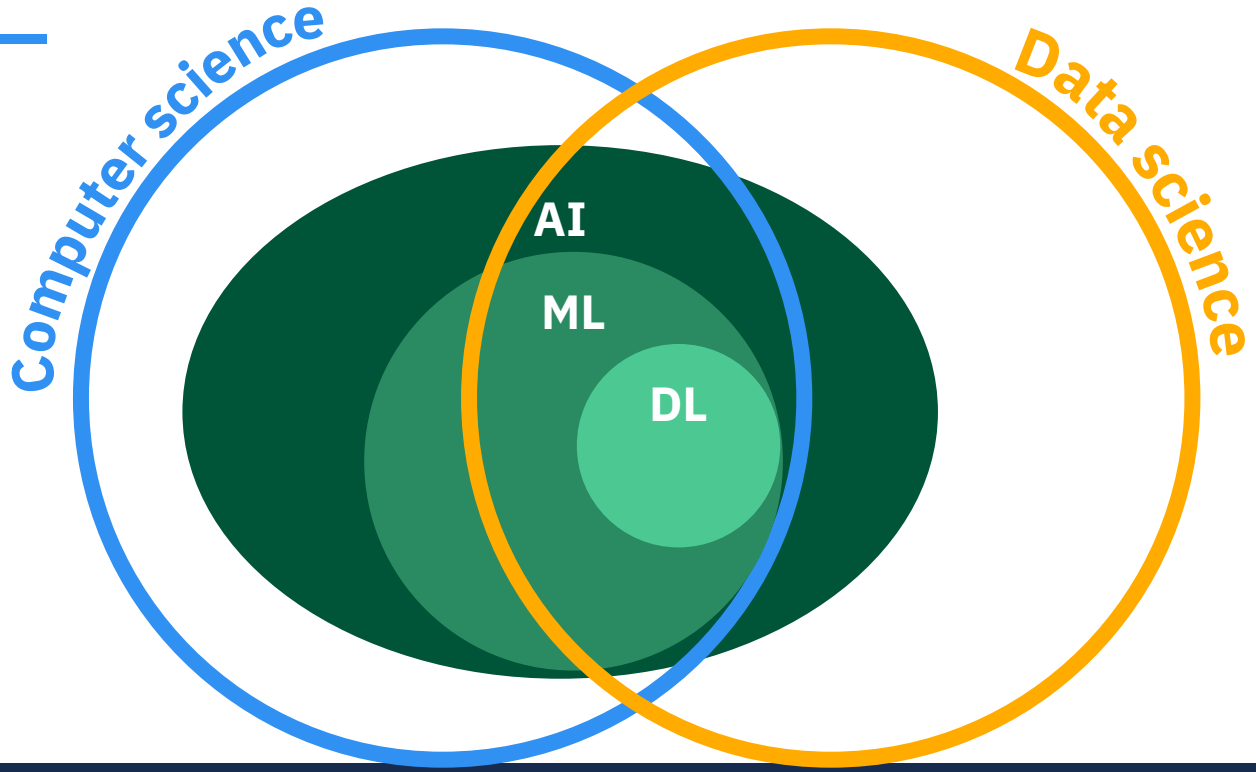
AI Ecosystem



Automatically learning from large amounts of data

DL = deep learning

AI Ecosystem

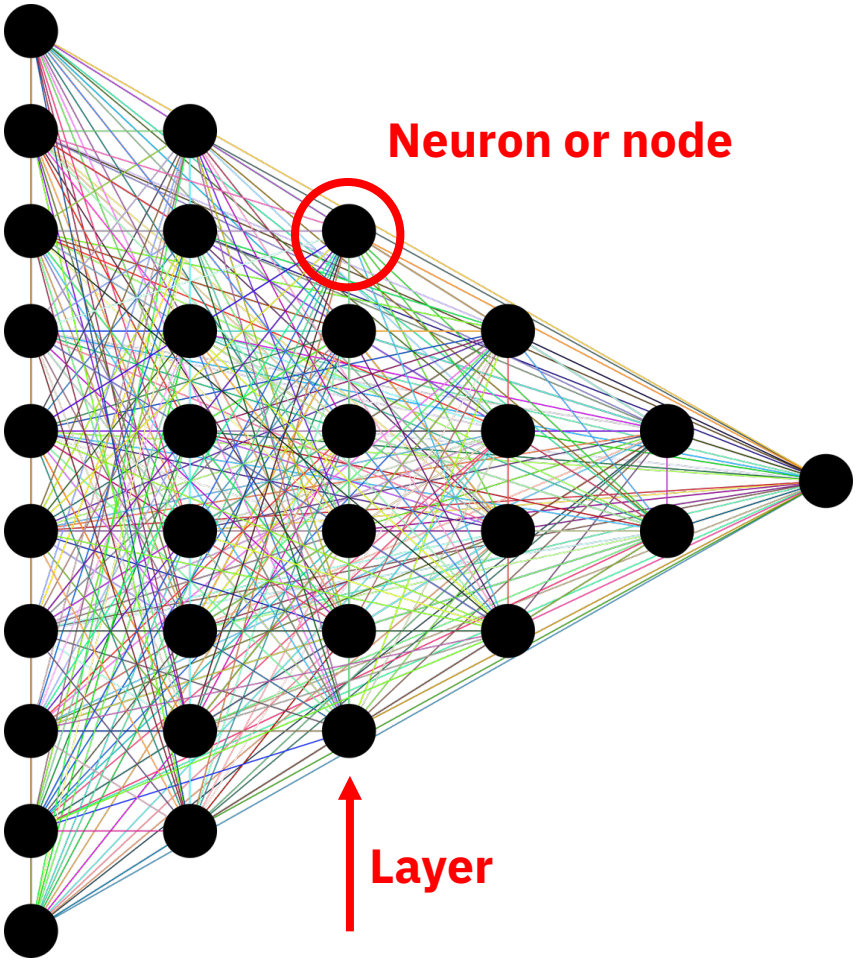


Machine Learning

Learning patterns from data and **improving performance** without being explicitly programmed

Inputs	(Semi-) Structured data
Processing	Algorithmic model
Outputs	Predictions, classifications, suggestions

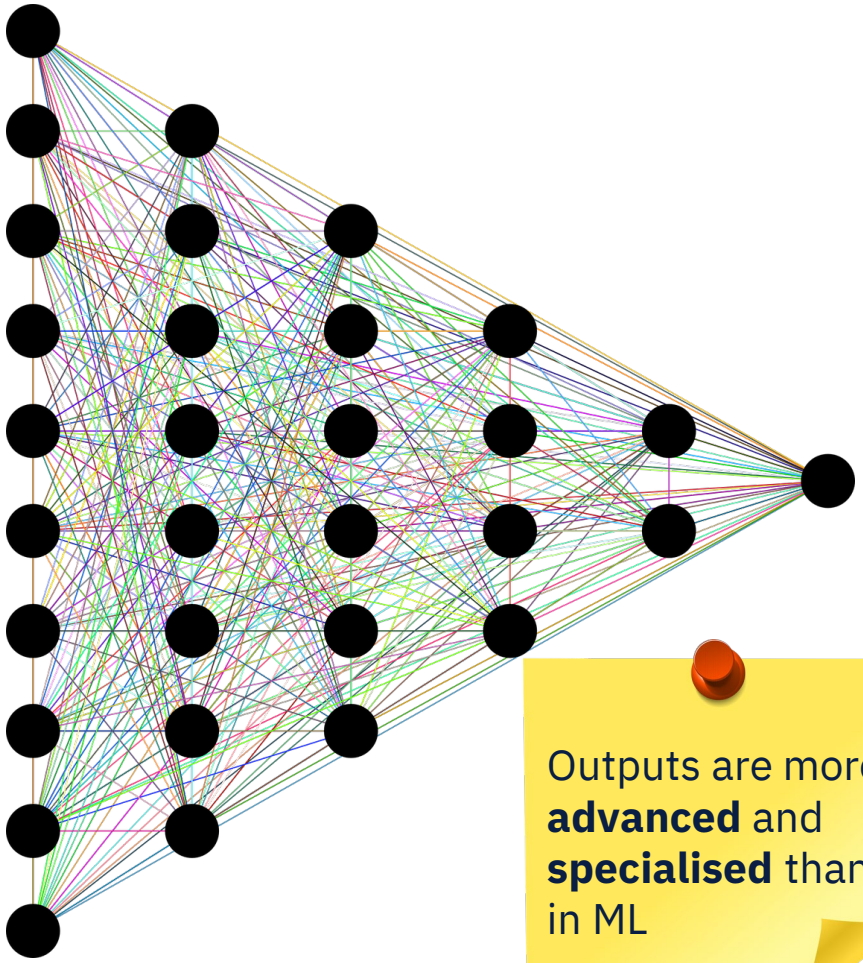
```python
def sort_chemicals(chemicals):
    """
    Sort chemicals into CWC Schedules based on their properties.

    :param chemicals: List of dictionaries, each containing the name and properties of a
                      Example: [{"name": "Sarin", "toxicity": "High", "legitimate_use": '
    :return: A dictionary categorizing chemicals into Schedules 1, 2, and 3.
    """
    # Create empty lists for each schedule
    schedules = {"Schedule 1": [], "Schedule 2": [], "Schedule 3": []}

    for chemical in chemicals:
        name = chemical["name"]
        toxicity = chemical["toxicity"]  # e.g., "High", "Medium", "Low"
        legitimate_use = chemical["legitimate_use"]  # e.g., "High", "Medium", "Low"

        # Classify chemicals into schedules
        if toxicity == "High" and legitimate_use == "Low":
            schedules["Schedule 1"].append(name)
        elif toxicity in ["High", "Medium"] and legitimate_use in ["Medium", "Low"]:
            schedules["Schedule 2"].append(name)
        else:  # Default to Schedule 3
            schedules["Schedule 3"].append(name)

    return schedules
```



Deep Learning

Automatically learning patterns from **large amounts of data**, especially for **complex tasks**, using multi-layered neural networks

Inputs	Unstructured data
Processing	Neural network model
Outputs	Predictions, classifications, generative output



Outputs are more **advanced** and **specialised** than in ML

Deep Learning

Automatically learning patterns from **large amounts of data**, especially for **complex tasks**, using multi-layered neural networks

Inputs	Unstructured data
Processing	Neural network model
Outputs	Predictions, classifications, generative output

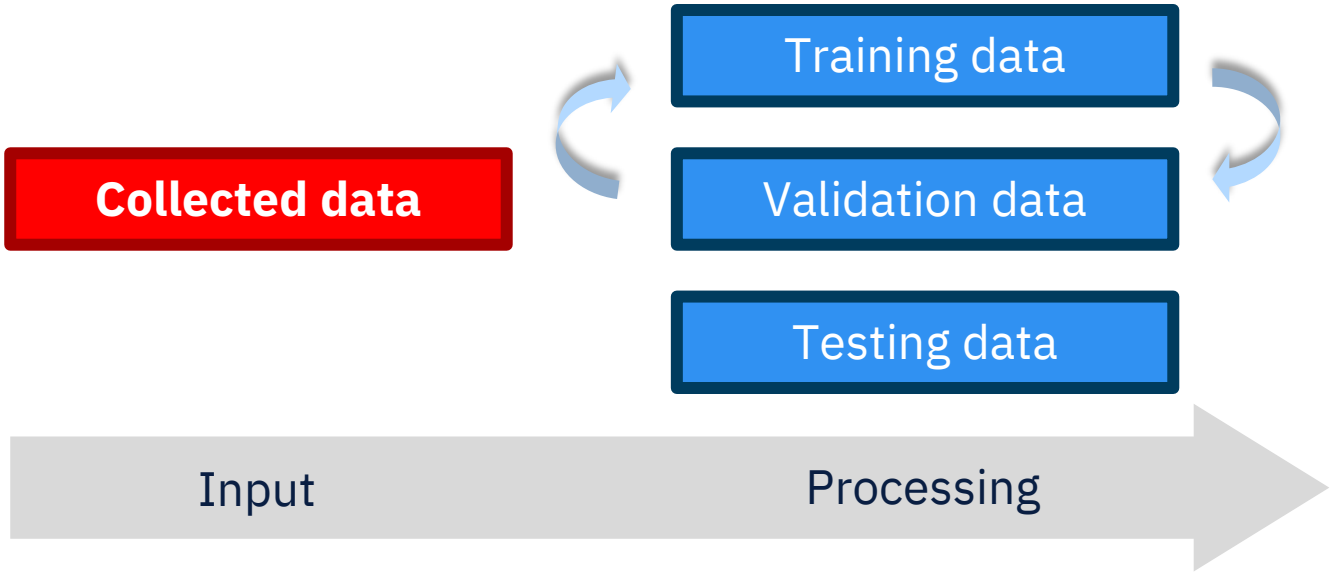
Training Process

“Garbage in, garbage out”

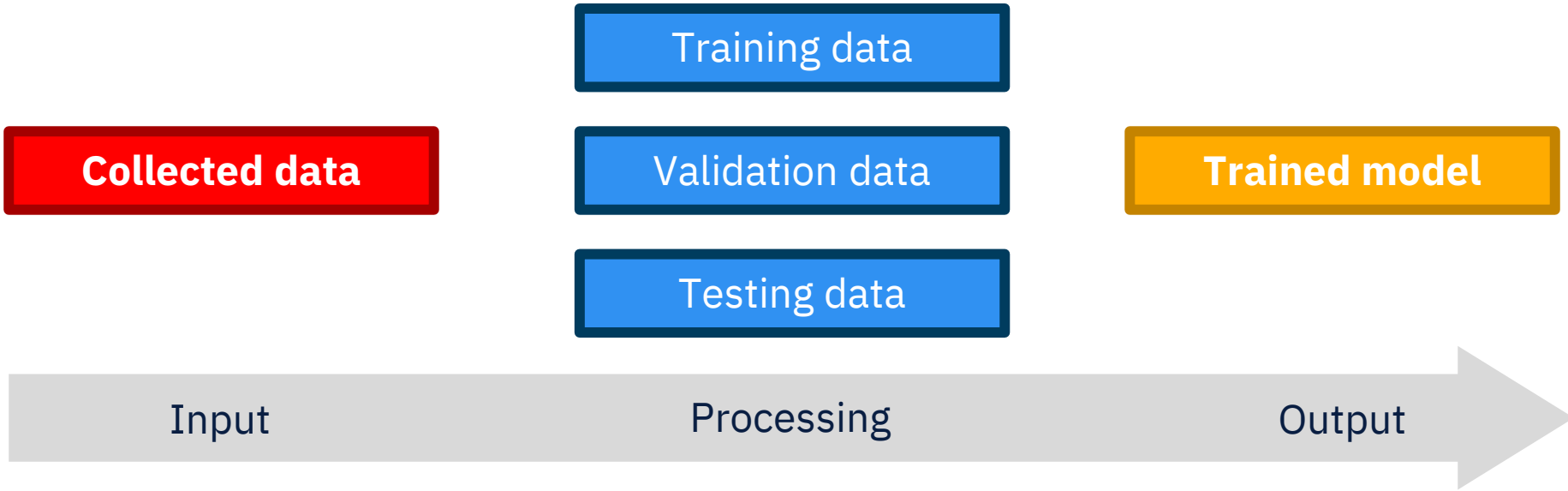
Collected data

Input

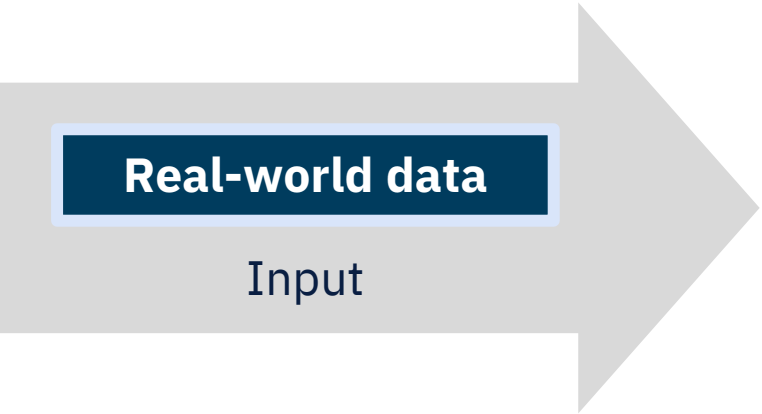
Training Process



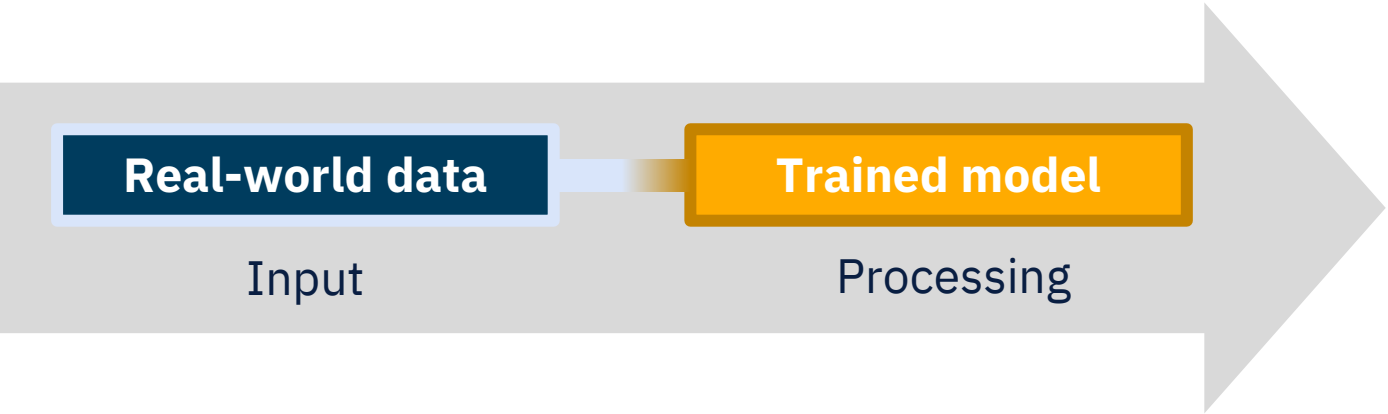
Training Process



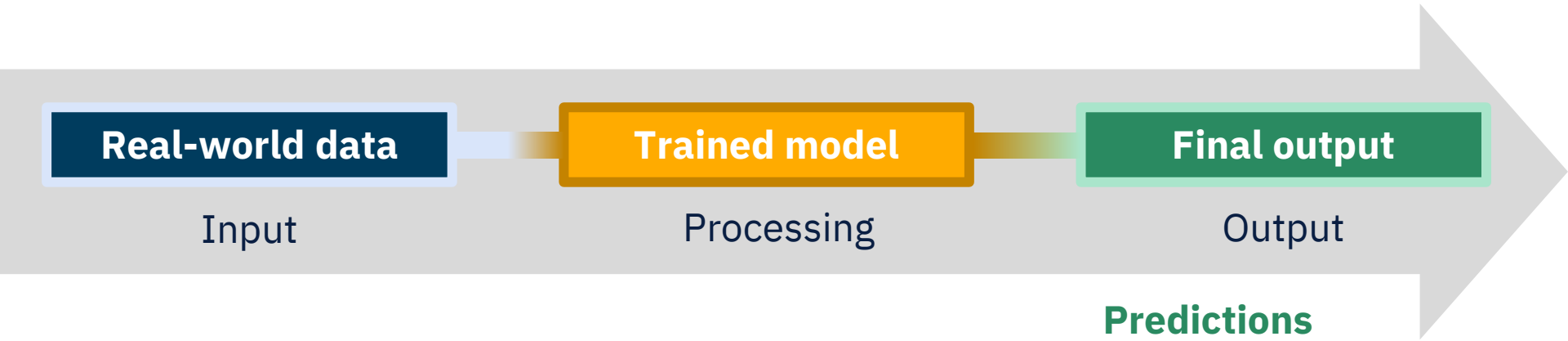
Deployment Process

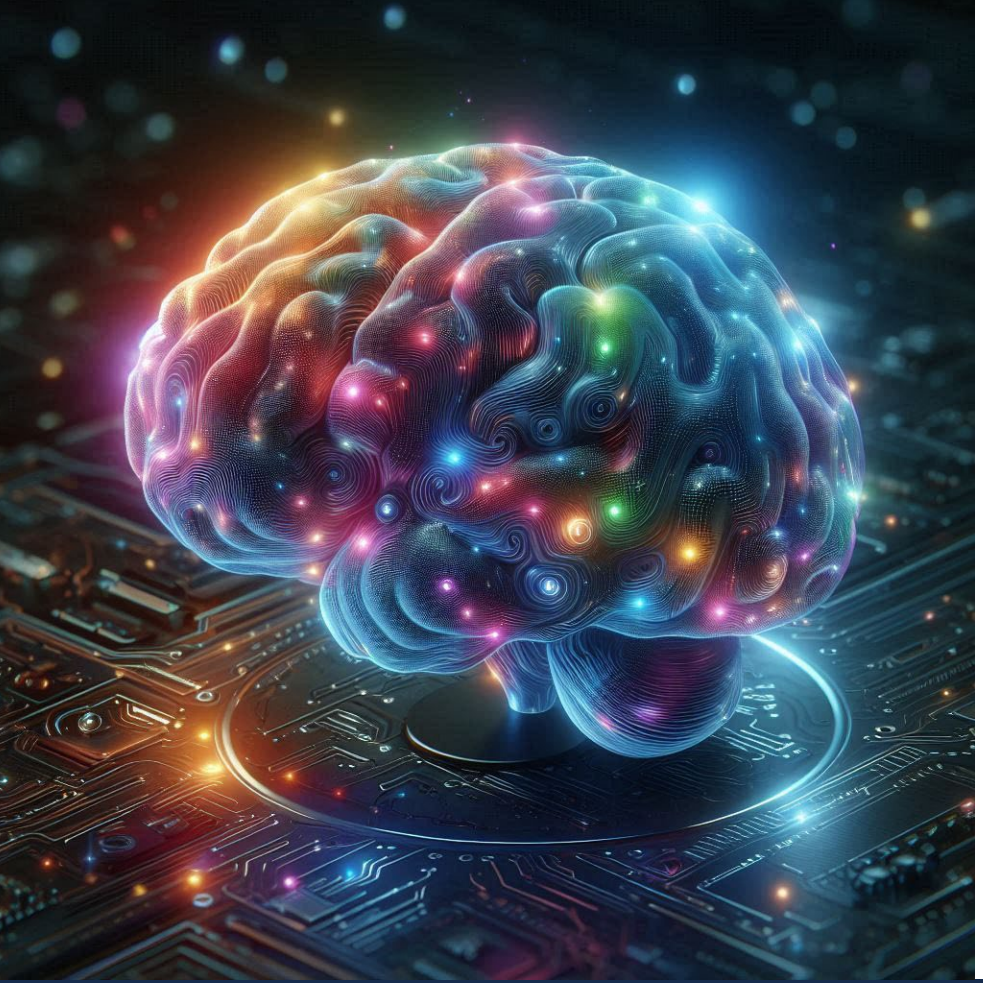


Deployment Process



Deployment Process





Applications of AI

Autocorrect

Email filtering

Virtual assistants

Social media feeds

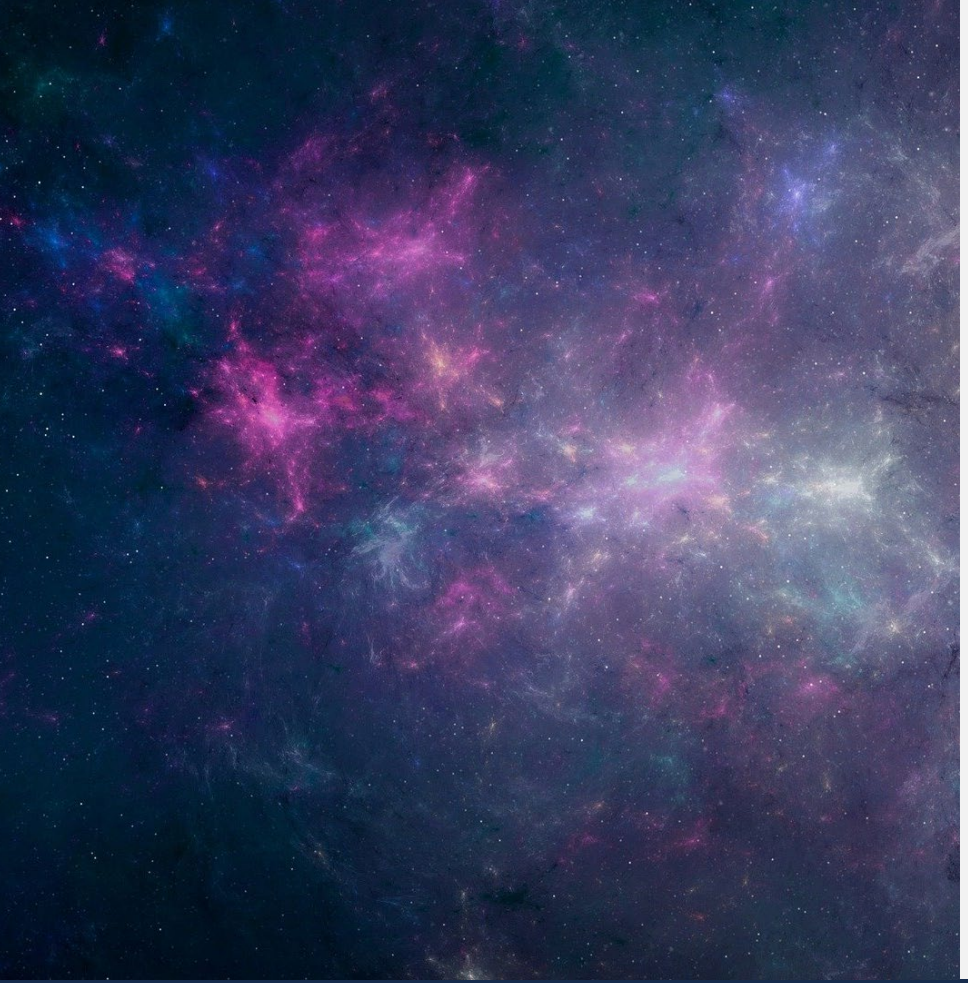
Search engines

Shopping recommendations

Navigation apps

Smart home devices


02
AI in
Chemistry
KLING AI



Chemical Discovery

Addressing global challenges and improving quality of life

Chemical Discovery

Approximately

**1,000,000,000,000,000,000,
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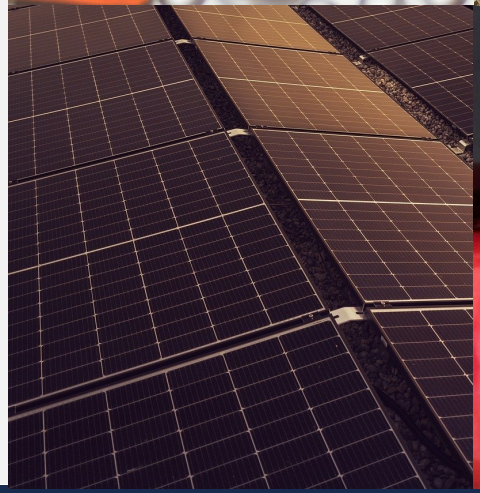
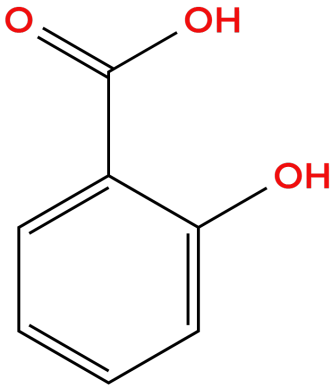
small organic molecules
in chemical space



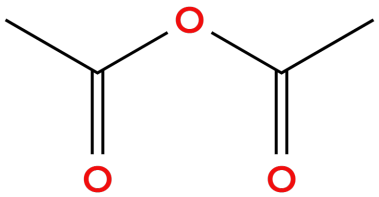
Synthesis Planning

Reagents

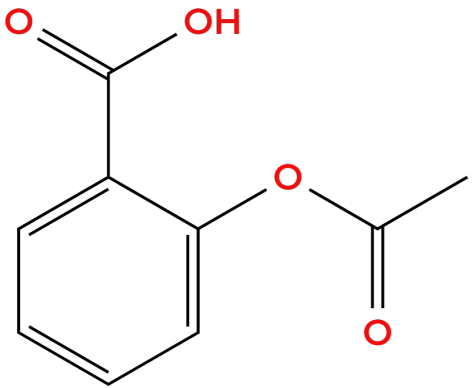
Products



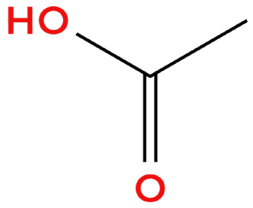
Salicylic acid



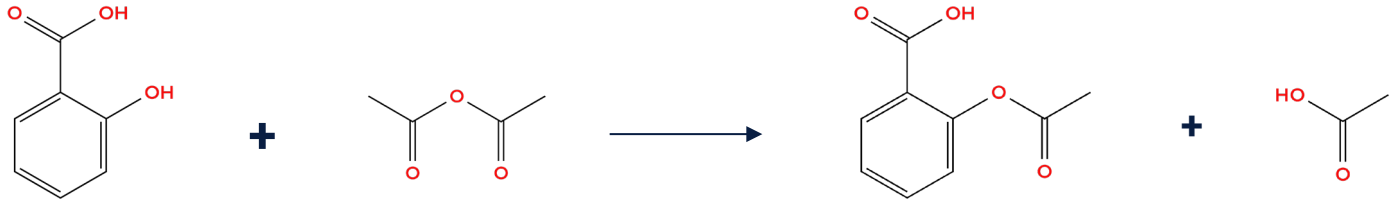
Acetic anhydride



Aspirin



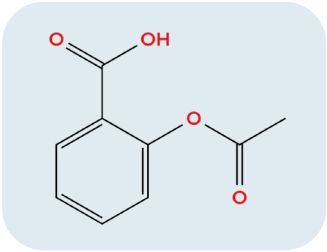
Acetic acid



Retrosynthesis

Synthesis Planning

Forward prediction

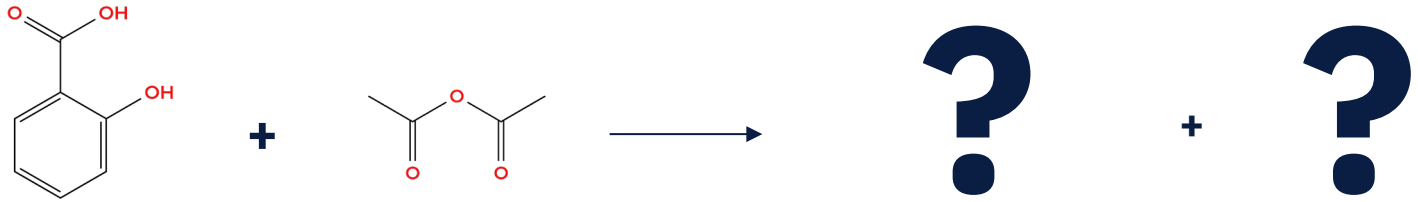
? + ? → 

Retrosynthesis

- Working **backwards from a target molecule** to identify possible reagents
- Deconstructs target into simpler components
- AI predicts feasible disconnections

Synthesis Planning

Forward prediction



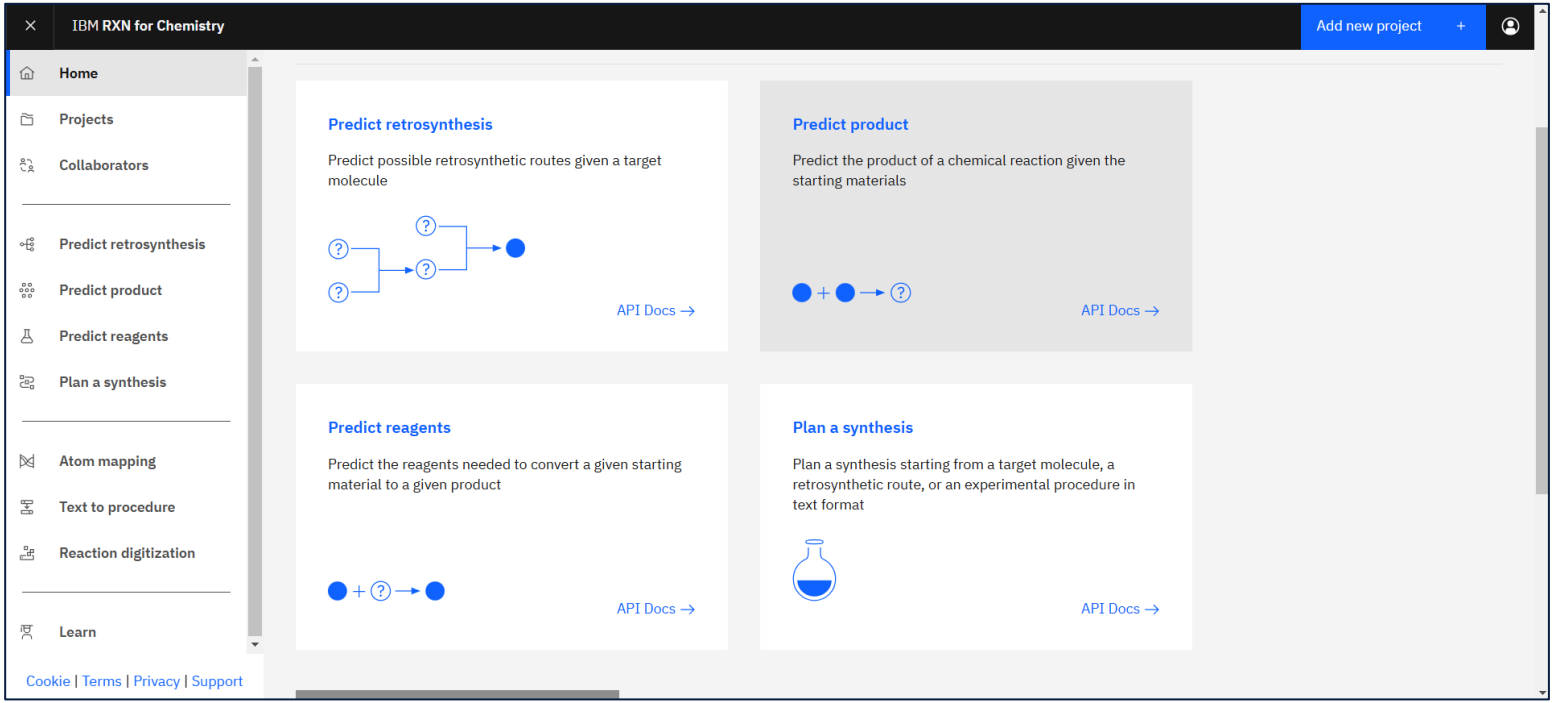
Retrosynthesis

Synthesis Planning

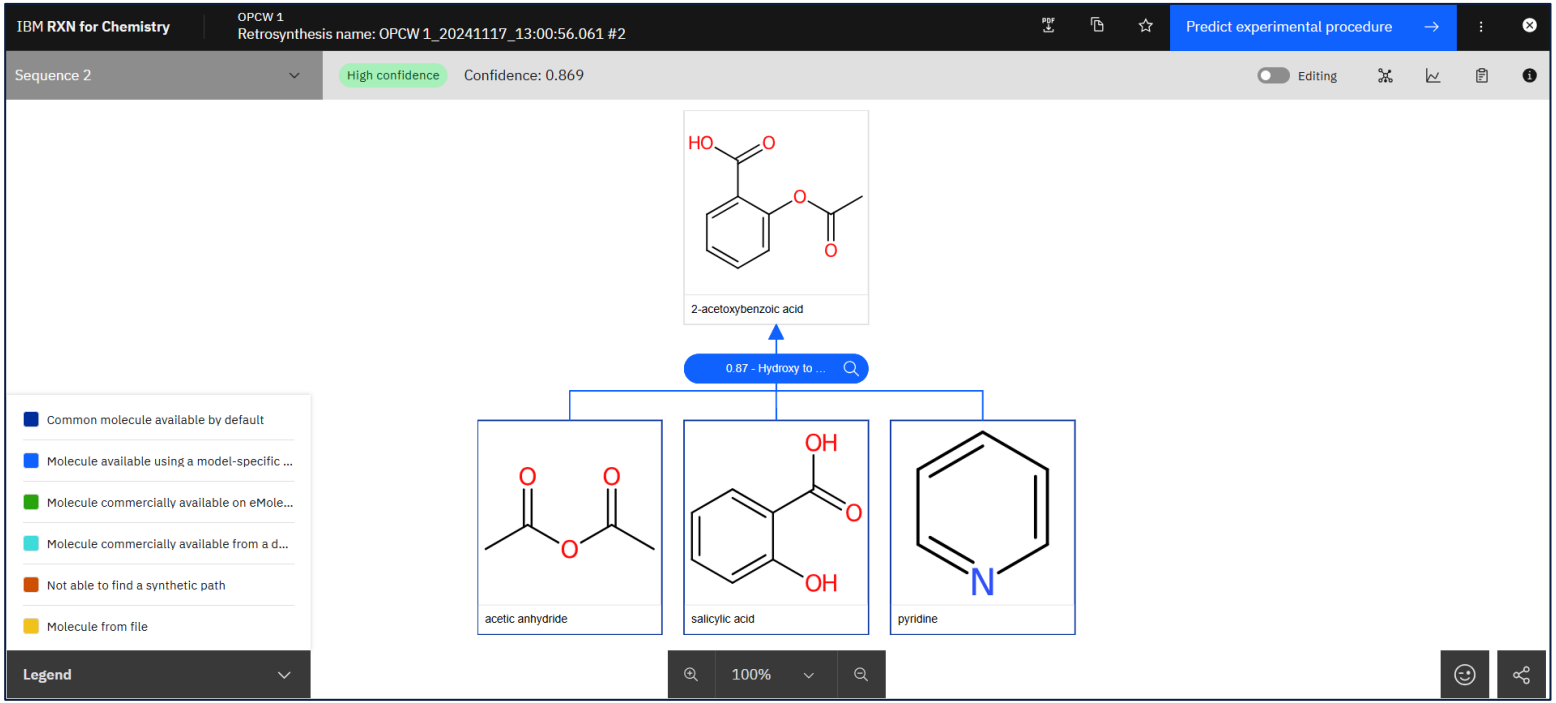
Forward prediction

- Working **forwards from the reagents** to identify reaction outcomes
- Constructs target from available reagents
- AI predicts possible products and optimise reaction conditions

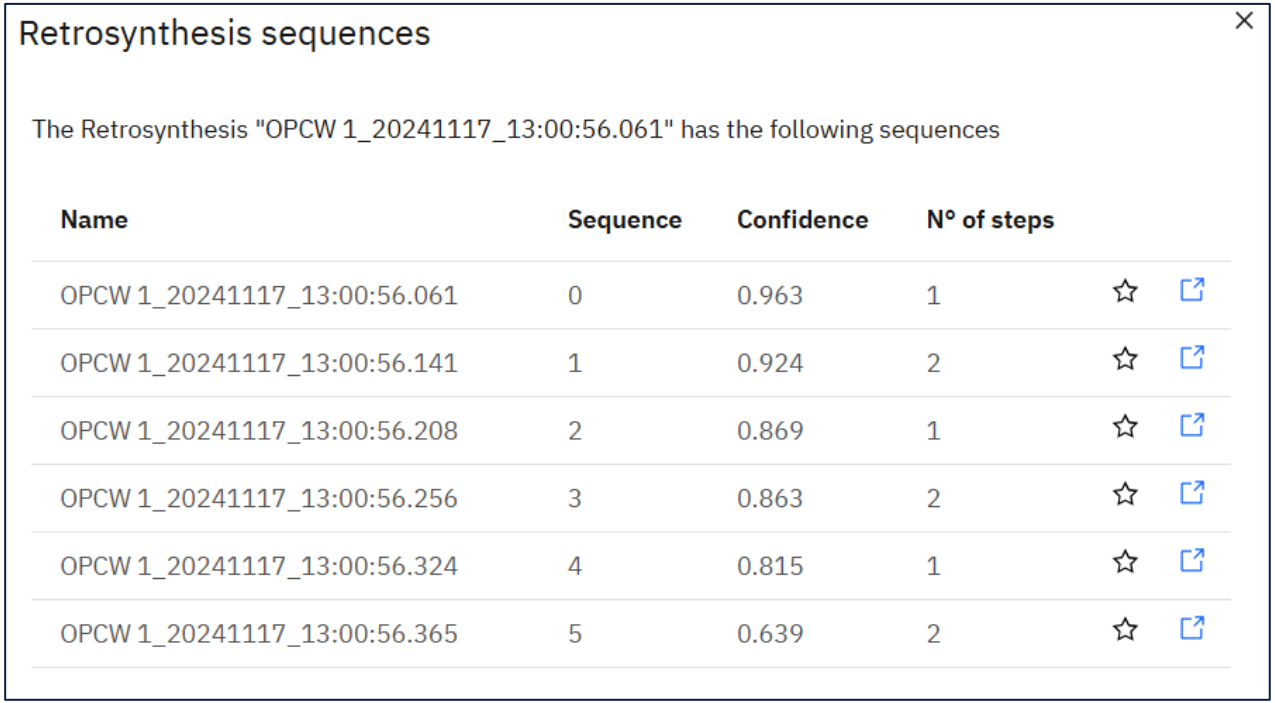
Synthesis Planning Tools



Synthesis Planning Tools



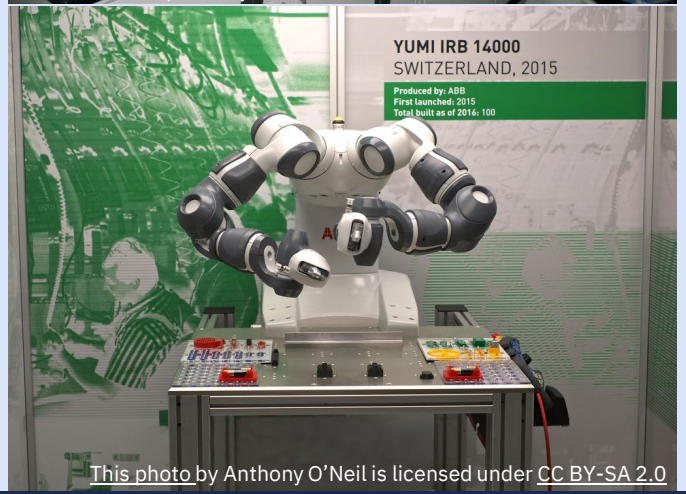
Synthesis Planning Tools



Robotics and Automation

Laboratory robots and “cobots”

From automated equipment and robotic arms…



Laboratory robots and “cobots”

…to self-driving labs

https://www.youtube.com/watch?v=srC3c6lQL2w

Cloud labs

Emerald Cloud Lab

https://www.youtube.com/watch?v=SJ0ZP-xEkBM

Chemical Safety

- Mixed reality training
- Predictive maintenance
- Real-time monitoring
- Toxicity prediction
- Improved risk assessment models
- Hazardous chemical substitution

Chemical Detection, Identification, and Forensics

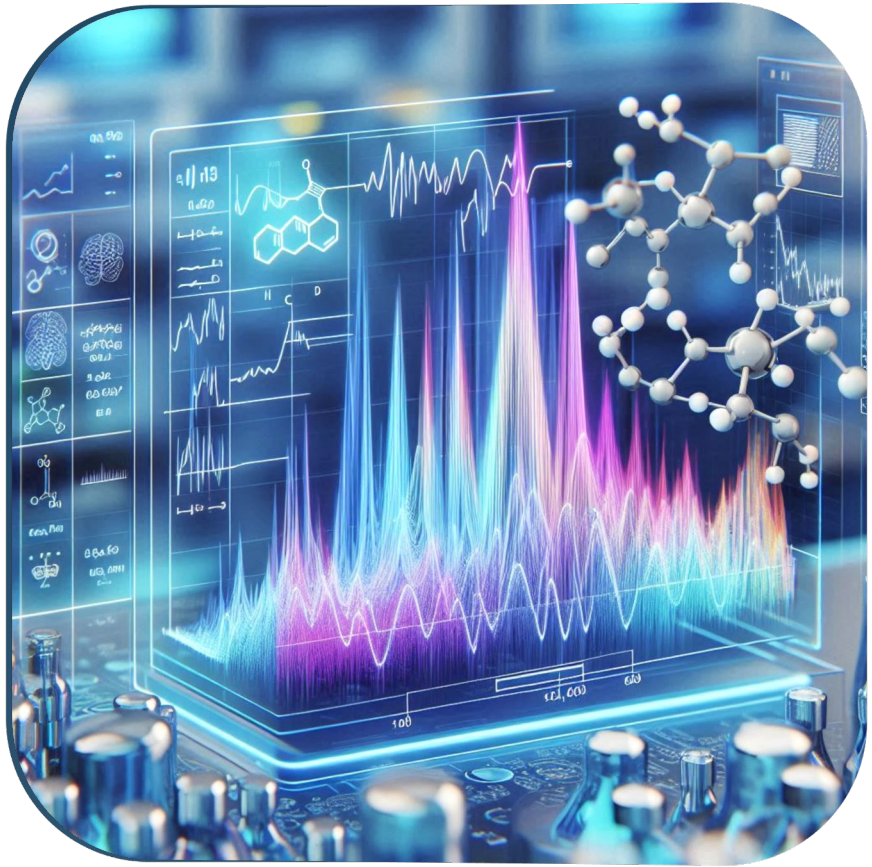
AI is improving:

- speed
- accuracy
- reliability

Data analysis and pattern recognition

- Analyse vast datasets rapidly
- Discern patterns, correlations, and anomalies
- Identify compounds or trace substances with high accuracy and speed

Time needed for analysis and interpretation



Real-time monitoring and detection

- Analysis of sensor data and make immediate decisions
- Predictive alerts of chemical threats
- Identification of exposure risks in a chemical plant

Personnel safety

04

AI and the OPCW

Scientific Advisory Board 2024

S&T under review

- **Independent** advisory board
- 25 experts
- Report on developments to Review Conferences

(POTENTIAL) OPPORTUNITIES

- Increase safety
- Optimise resources
- Streamline processes
- Enhance risk assessment
- Generate training scenarios
- Strengthen capacity building
- Improve detection capabilities
- Reinvigorate MedCM research
- Leverage open-source data
- Identify emerging threats
- Monitor advances in S&T
- Design new materials
- Predict spectral data
- Fuse spectral data

(POTENTIAL) RISKS

- Predict toxicity
- Optimise production
- Disguise illicit purchases
- Spread misinformation
- Identify novel syntheses
- Design hazardous chemicals
- Proliferate sensitive knowledge
- Hack chemical control systems
- Provide fast access to info
- Reduce technical barriers
- Optimise dissemination
- Identify vulnerabilities
- Circumvent controls
- Evade detection

Artificial Intelligence

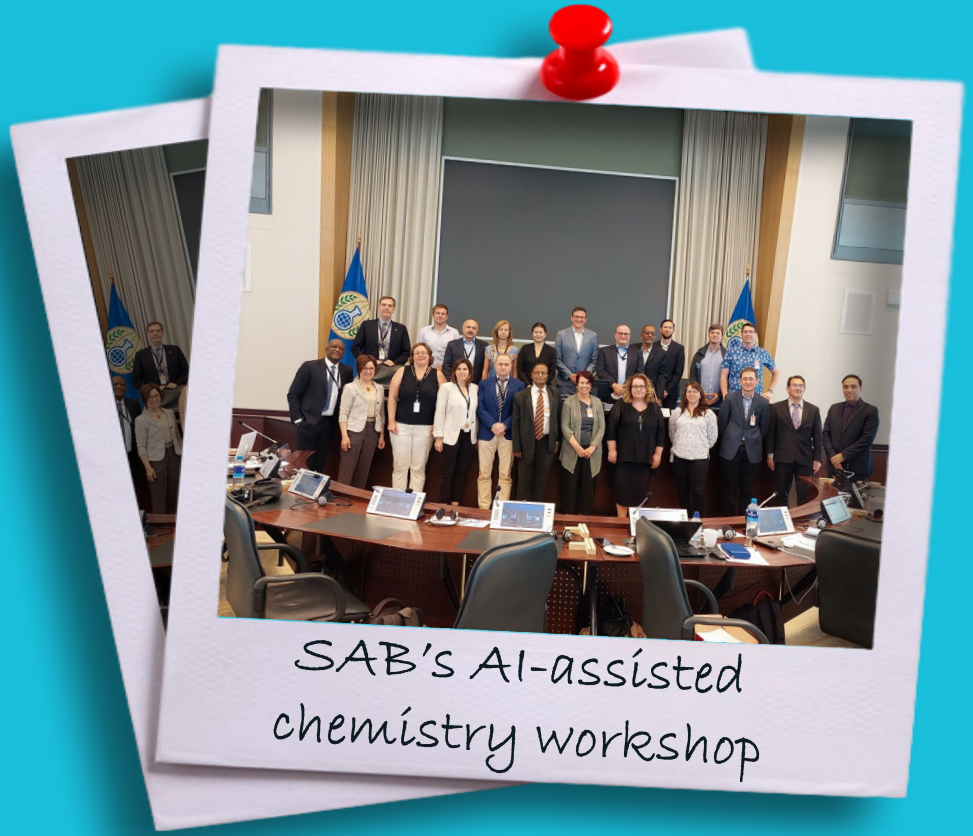
“

The OPCW should closely monitor the rapid development in AI-assisted chemistry and machine learning and consider not just the potential risks that it poses, but also the opportunities it presents

SAB recommendation

Credit: University of Liverpool

OPCW HQ



SAB's AI-assisted chemistry workshop

2021

June

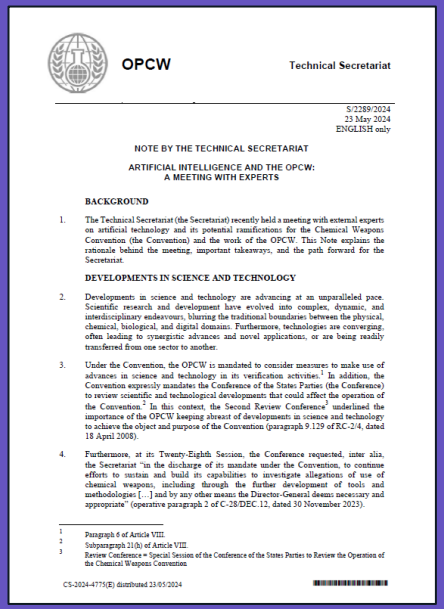
2022

2023

April

OPCW HQ

AI Meeting with Experts



OPCW Technical Secretariat

S/2289/2024
23 May 2024
ENGLISH only

NOTE BY THE TECHNICAL SECRETARIAT

ARTIFICIAL INTELLIGENCE AND THE OPCW:
A MEETING WITH EXPERTS

BACKGROUND

1. The Technical Secretariat (the Secretariat) recently held a meeting with external experts on artificial technology and its potential ramifications for the Chemical Weapons Convention (the Convention) and the work of the OPCW. This Note explains the rationale behind the meeting, important takeaways, and the path forward for the Secretariat.

DEVELOPMENTS IN SCIENCE AND TECHNOLOGY

2. Developments in science and technology are advancing at an unparalleled pace. Scientific research and development have evolved into complex, dynamic, and interdisciplinary endeavours, blurring the traditional boundaries between the physical, chemical, biological, and digital domains. Furthermore, technologies are converging, often leading to synergistic advances and novel applications, or are being readily transferred from one sector to another.

3. Under the Convention, the OPCW is mandated to consider measures to make use of advances in science and technology in its verification activities.[1] In addition, the Convention expressly mandates the Conference of the States Parties (the Conference) to review scientific and technological developments that could affect the operation of the Convention.[2] In this context, the Second Review Conference[3] underlined the importance of the OPCW keeping abreast of developments in science and technology to achieve the object and purpose of the Convention (paragraph 9.129 of RC-2/4, dated 18 April 2008).

4. Furthermore, at its Twenty-Eighth Session, the Conference requested, inter alia, the Secretariat "in the discharge of its mandate under the Convention, to continue efforts to sustain and build its capabilities to investigate allegations of use of chemical weapons, including through the further development of tools and methodologies […] and by any other means the Director-General deems necessary and appropriate" (operative paragraph 2 of C-28/DEC.12, dated 30 November 2023).

1 Paragraph 6 of Article VIII.
2 Subparagraph 21(h) of Article VIII.
3 Review Conference = Special Session of the Conference of the States Parties to Review the Operation of the Chemical Weapons Convention

CS-2024-4775(E) distributed 23/05/2024

S/2289/2024, dated 23 May 2024

2023

April

2024

June

2024

Berlin, Germany

AI and WMD

Keynote address, rethinkingarmscontrol.org

April
2024

June
2024

October
2024

Rabat, Morocco

Global Conference

Role of Artificial Intelligence in Advancing the Implementation of the CWC

- Enhance understanding of AI
- Contextualise developments
- Inform future policy discussions

Topics included chemistry, policy, security, and opportunities and challenges to implementation of the CWC

Kingdom of Morocco

June 2024

October 2024

January 2025

Rabat, Morocco

Global Conference

190 delegates

46 States Parties

Available on Catalyst

June 2024

October 2024

January 2025

OPCW HQ

October

2024

Temporary Working Group on AI

Objectives

Understand the impact of AI on the CWC and identify the risks and opportunities for its implementation

Duration of **1 year**

Composition

Approximately 15 members

January

2025

OPCW HQ

October

2024

Temporary Working Group on AI

Data prediction and generation

Automated synthesis

Synthesis planning

Data curation

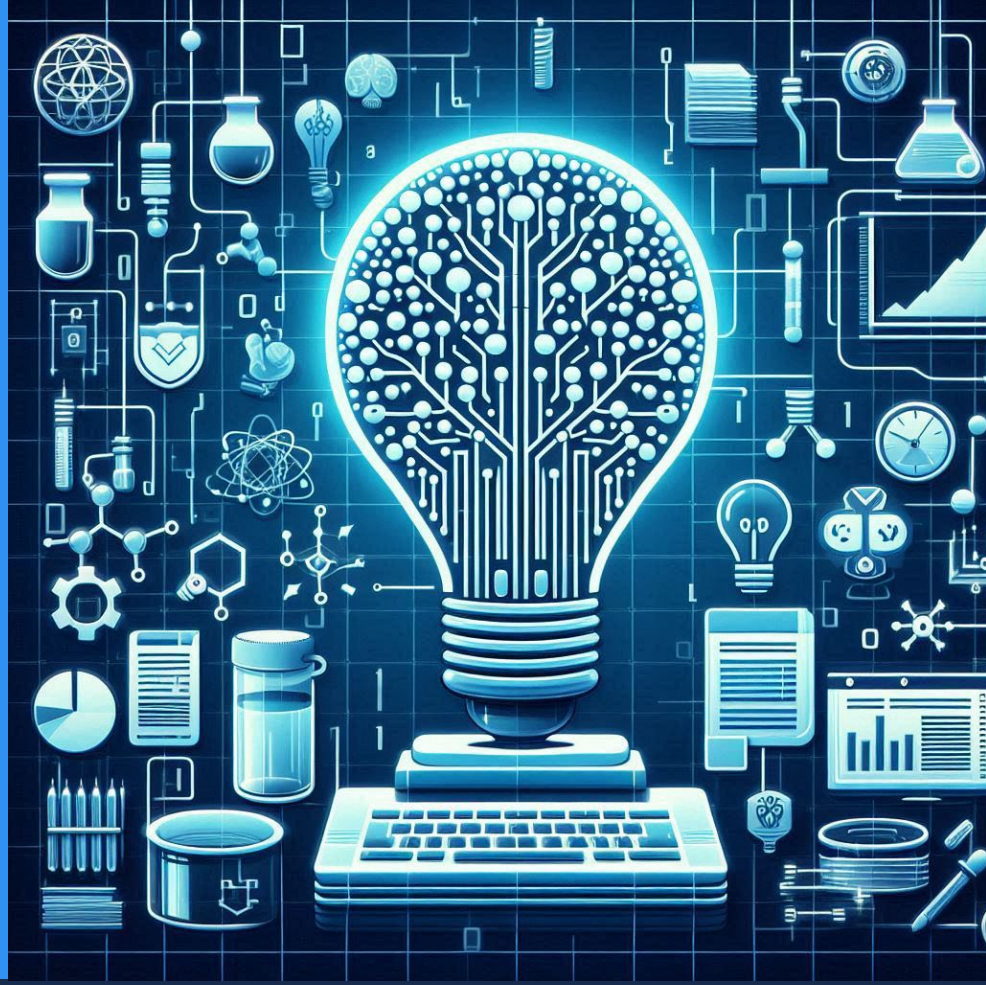
Data fusion

January

2025

OPCW AI Research Challenge

Crowdsourcing innovative AI solutions to assist the OPCW



AI Challenge

Identify how AI can be used to **strengthen the OPCW's capabilities** and **increase its readiness** to address current and future challenges

22 proposals received

4 proposals, up to €65,000 each

Duration of 1 year

Next Steps

Summary

1

AI produces diverse outputs and has a broad range of applications

2

In chemistry, AI:

- accelerates progress
- increases accuracy
- improves process optimisation
- enhances safety

3

The OPCW is making progress in identifying the potential risks and opportunities AI poses to the Convention