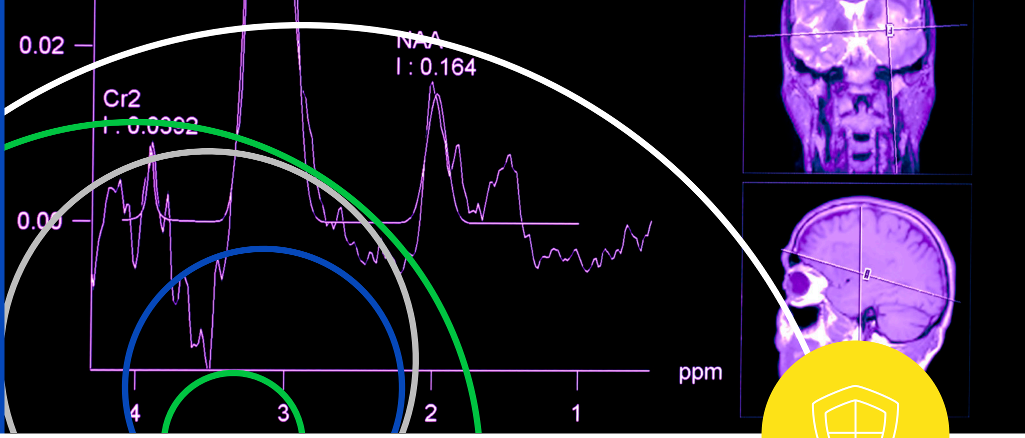


Project Results

Spectralligence

Spectral analysis with artificial intelligence

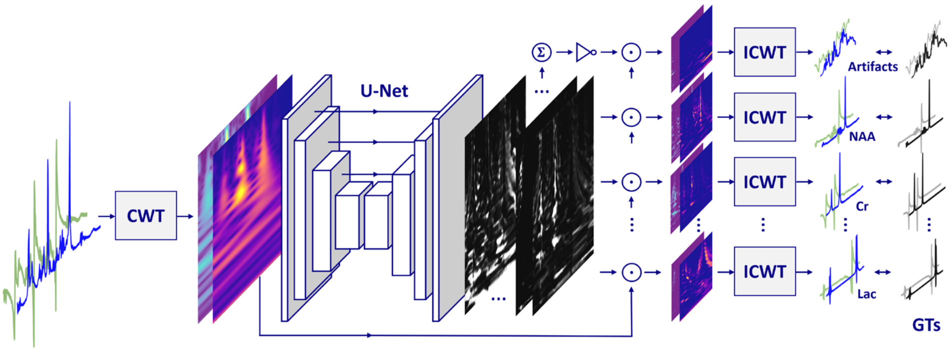
To reduce expert dependence in spectroscopy, the ITEA project Spectralligence (Spectral Analysis in life sciences and materials sciences through Artificial Intelligence) combined artificial intelligence (AI) and machine learning (ML) techniques with spectral analysis across broad domains.

Molecular and atomic spectroscopy refers to a set of technologies that use the electromagnetic spectrum to generate unique fingerprints for molecular structures. This field is seeing rapid technological development via component miniaturisation and increased embedded processing power while also expanding into areas like personalised medicine and environmental surveillance. However, the acquisition and interpretation of spectral data currently requires highly-trained experts. A reduction in human dependency is therefore needed to further develop the field.

Spectalligence offers a solution by augmenting innovations in micro-electronics and component miniaturisation with cross-domain-validated neural networks for spectral analysis, serving as industrial-grade embedded AI technologies for one-click spectral characterisation in the materials and life sciences. Four major advancements were targeted within the project: (1) simulated data for spectral reconstruction and denoising with AI/ML; (2) improved component detection in polluted water matrices with AI/ML; (3) AI/ML-based parcel screening automation using neutron spectroscopy; and (4) direct quantification of brain metabolites. Through this, Spectralligence provides a foundation to augment and replace expert users in data workup for various molecular and atomic spectroscopy technologies.

Technology applied

As an explorative project at the early TRLs, Spectralligence focused on general availability and open-source approaches, such as leveraging the Osprey platform as a basis to include models developed in Spectralligence (like WAND for artifact removal). However, spectroscopy is often used in highly-regulated environments like healthcare, necessitating simulation-based data augmentation and generation. In its work on the design, training and validation of a physics-informed AI methodology for spectroscopy analysis, the project therefore focused on digital phantoms, digital reference objects and data generation. This has enabled the use of out-of-domain, non-privacy-sensitive data to train ML models for enhanced spectral reconstruction, including denoising and artifact removal, and helps address challenges such as low spectral signal-to-noise ratio, overlapping metabolites and high acquisition times. The result is novel neural network designs and training strategies for spectral quantification and analysis, as well as novel data-driven simulation tools to enrich real measurements.



^ Spectralligence's WAND Architecture for hybrid classical-Deep Learning spectral analysis

Regarding AI for spectral-informed material characterisation, Spectralligence targeted application development and one-click workflow integration in three domain-specific use-cases. In each of these, the spectroscopic workflow was defined and new architectures and enhanced spectral analysis neural networks were investigated. For magnetic resonance spectroscopy, manual steps by a trained operator can be replaced with an AI-based decision algorithm that provides users with optimal outcomes (such as a brain tumour's status) regardless of a lack of knowledge of the specific system. For neutron-induced gamma-ray emission spectroscopy, an AI-based decision algorithm processes raw spectral data and provides deconvoluted data to a trained network to estimate the presence of threat materials. For optical spectroscopy, AI-based algorithms provide accurate quantitative data on metal concentrations in water to remove manual calibration and analysis by operators.

Making the difference

Despite a lack of public awareness, spectroscopy has enormous implications in many domains. Spectralligence's key achievement is therefore its foundational work in bringing AI/ML to this field, having trained models on simulated data in three important domains and created two models/steps proposed for inclusion in open-source packages – all against a starting point of zero. The individual use-cases have also seen breakthrough results. For neutron-induced gamma-ray emission spectroscopy, for instance, Spectralligence was able to accurately identify a range of products (such as explosives and drugs) in parcels and suitcases with a 3-4x better false alarm rate than current X-ray-based security screening. In optical spectroscopy, meanwhile, convolutional neural network-based calibration models were created that perform equally well to manual models but with >90% time savings via AI.

While these results have been achieved at TRLs 3-4, Spectralligence has also made strong progress towards exploitation. Whereas magnetic resonance imaging typically detects protons in water due to their abundance and sensitivity, other nuclei (like phosphorus and fluorine) can also be visualised using spectroscopy. Within the project, Philips applied ML advances originally developed for proton imaging to improve the signal-to-noise ratio of X-nuclei imaging, reaching TRLs 4-5. They have now partnered with Polarean to co-sell hyperpolarised xenon imaging, used mainly for lung visualisation. Philips is unique in having achieved full regulatory approval for this, offering them a strong competitive advantage on the path to clinical adoption.

The future

Given the widespread benefits of spectroscopy, the adoption of Spectralligence's innovations could have a major societal impact. For example, this technology can be used to identify all forms of per- and polyfluoroalkyl substances (PFAS), some of which are banned but escape detection via reformulation. This could improve environmental pollution monitoring, particularly if linked to wastewater analysis. In medicine, a key application would be extending non-ionising radiation-based diagnostics, especially for new oncology drugs that can cost EUR 5,000-20,000 per dose, thereby assessing their effectiveness early on to reduce side effects and costs while improving patient outcomes. For Spectralligence, the next step is collaboration with the Innovative Health Initiative (IHI) that focuses on the later TRLs and clinical adoption, through which the project aims to help make such revolutions a reality.

Major project outcomes

Dissemination

- Seminal Review paper on the role of AI in clinical MR Spectroscopy.
- 2 publications in Magnetic Resonance Medicine and Metabolites, 4 pre-publications available at arxiv.
- 8 presentations at conferences like ISMRM.
- Workshop with 10 players in the spectroscopy & AI/ML domain.

Exploitation (so far)

- Digital MultiNuclei MR Spectroscopy platform, allowing for improved SNR spectroscopy in MRI.
- 129Xe partnership Philips-Polarean, co-selling hyperpolarised xenon imaging, used mainly for MR lung visualisation.
- Dual-tuned RF coils partnerships with a.o. Rapid Medical and Tesla DC.

Standardisation

- Open-Source reconstruction & processing, Digital Reference Phantom.
- Participation in IEC/ISO and ASTM committees related to (multi-nuclear) MR safety.

Spin offs

- Forever Analytical Solutions (FAS) Europe – advancing Dynaxion's innovations.

Spectralligence

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Partners

Finland

- Sensmet Oy

The Netherlands

- Dynaxion
- Eindhoven University of Technology
- Maastricht University Medical Center
- Philips Medical Systems Nederland BV
- UMC Utrecht

Project start

July 2021

Project end

October 2024

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https://spectralligence.eu/

https://itea4.org/project/spectralligence.html