MASTER FORENSIC SCIENCE - LITERATURE THESIS

Title	: AI and ML in Mass Spectrometry: Current Status and Emerging Trends
Keywords	: Mass Spectrometry, predictions, Artificial Intelligence, Machine Learning
Forensic Expertise Area	: Mass Spectrometry, Identification of chemicals unknown to databases
Start Date	: to be discussed
Host Institute	: OPCW
Department/Team	: Laboratory
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Short Description

The integration of Artificial Intelligence (AI) and Machine Learning (ML) into analytical chemistry is rapidly transforming the way mass spectrometry (MS) data is interpreted and utilized. The idea for this literature review is to investigate the current status and emerging developments in the use of AI and ML for the prediction of mass spectra and the support of experimental MS data evaluation.

The review should evaluate the recent advances in algorithmic approaches—including deep learning, neural networks, and ensemble models—that enable accurate spectral prediction from molecular structures and enhance the identification of unknown compounds.

The review could also explore the role of AI/ML in automating data processing workflows, reducing human bias, and improving reproducibility in forensic investigations with special attention to the challenges of model validation, data quality, and interpretability, as well as the ethical and regulatory considerations surrounding the deployment of AI-driven tools in forensic contexts.

Key References

1) Recent Developments in Machine Learning for Mass Spectrometry https://doi.org/10.1021/acsmeasuresciau.3c00060

2) Deep Learning-Enabled MS/MS Spectrum Prediction Facilitates Automated Identification of Novel Psychoactive Substances https://doi.org/10.1021/acs.analchem.3c02413

3) Deep Learning-Enabled MS/MS Spectrum Prediction Facilitates Automated Identification of Novel Psychoactive Substances Machine Learning meets mass spectrometry: a focused perspective https://doi.org/10.48550/arXiv.2407.00117

Required/Recommended skills and expertise
- Mass Spectrometry
- AI/ML (at least interest in those tools)
- Organic Chemistry (nomenclature & basics)

Visuals

