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### Mikaela Radke

BForensic Science, BSc (Honours) Class l mikaela.radke@griffithuni.edu.au orcid.org/0009-0008-7263-9117

#### Summary

This PhD will focus on the development of methods for identification of a wide range of emerging and environmentally significant contaminants, pollutants and xenobiotics through chemical and toxicological monitoring. This will be achieved through the application of high-resolution mass spectrometry which allows for the identification of unknown compounds through the acquisition of accurate mass precursor ions and fragmentation patterns. Within environmental contaminant monitoring there exists an analytical contaminant gap characterised by a bias towards the identification of compounds using specific types of analytical techniques. This does not allow for a true representation of the extent of environmental xenobiotics to be determined as there are compounds that cannot be identified using standard analytical procedures. Therefore, novel separation techniques will be applied in conjunction with high-resolution mass spectrometry and effect directed analysis to identify compounds of environmental and toxicological relevance. The separation techniques of focus are supercritical fluid chromatography and mixed mode liquid chromatography which will be applied to non-targeted methodologies to identify compounds that are more likely to persist in the environment and therefore pose a larger threat to aquatic and human life.

Non-targeted analysis is an emerging field within analytical chemistry focusing on identification of known and unknown compounds by analysing all components of a sample. This differs from targeted chemical analysis, commonly used in environmental and toxicological monitoring, where samples are analysed based on compounds predicted to be within a sample which have known features that can be targeted and used for identification. This novel application of non-targeted methodologies with a wide range of effect directed analysis techniques for monitoring of compounds that give a toxic response within environmental samples will allow for more complete characterisation of emerging compounds of concern within Australia.

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### **Research Expertise**

- Analytical chemistry
- High-resolution mass spectrometry using the Qq-Orbitrap mass analyser
- Method development and validation