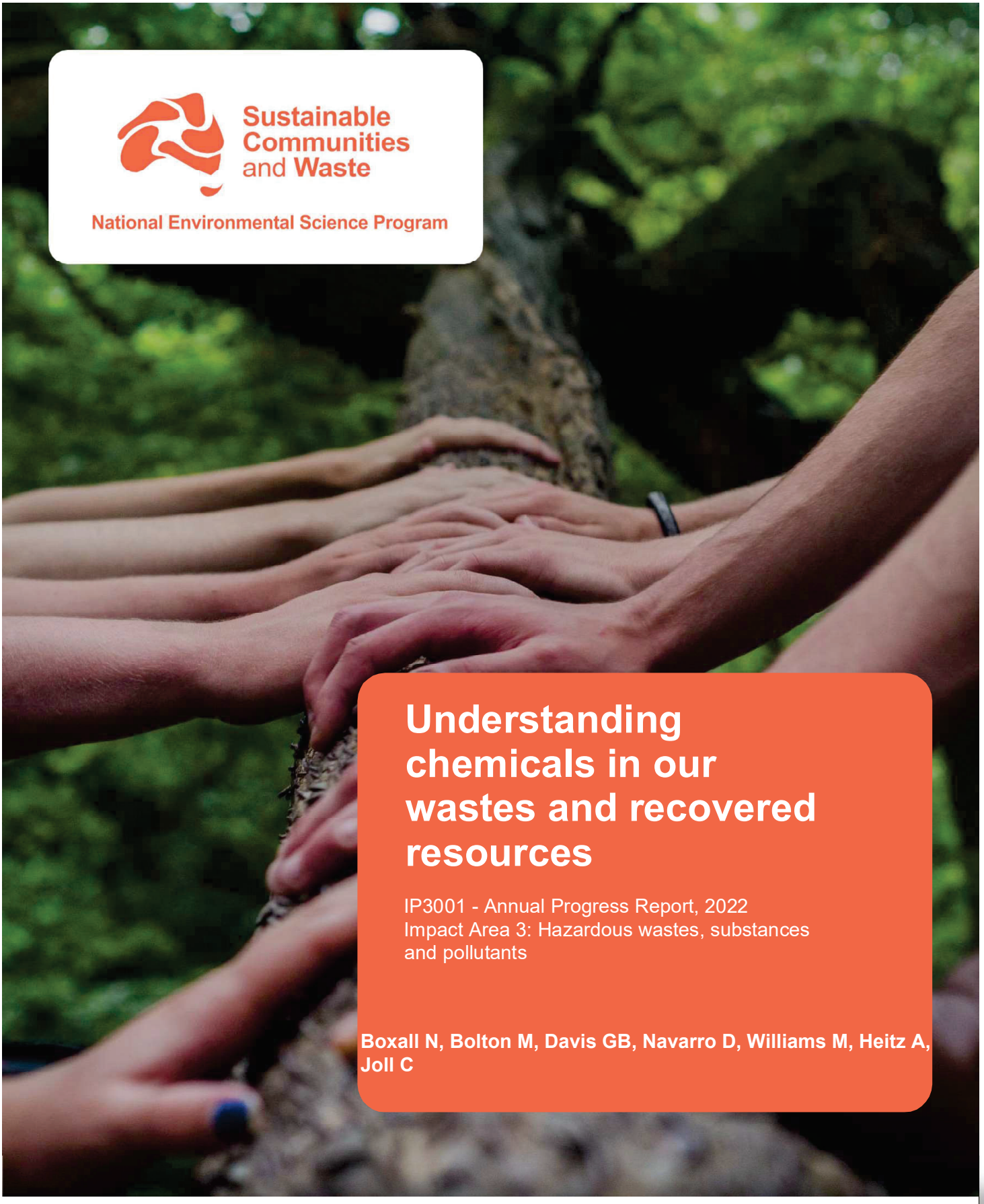

Sustainable Communities and Waste

National Environmental Science Program

Understanding chemicals in our wastes and recovered resources

IP3001 - Annual Progress Report, 2022
Impact Area 3: Hazardous wastes, substances and pollutants

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Project Team

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Related information

- Dataset: IP3_DS3 - Understanding chemicals in our wastes and recovered resources (Annual Progress Report, 2022).
- IP3.02_IP3002 – Interim guidance on sampling of complex materials

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Scope

This document has been prepared to fulfil the 2022 annual reporting requirements of Research Plan 2 (RP2) for the National Environmental Science Program (NESP), Sustainable Communities and Waste (SCaW) Hub, under Impact Area 3 (IP3), Hazardous Wastes, Substances and Pollutants work program.

Glossary of Terms

Term	Definition
Chemicals of concern	Chemicals that can have long-term adverse effects on humans or ecosystems
Chemical exposure	Concentration or amount of a particular agent that reaches a target organism, system, or (sub)population in a specific frequency for a defined duration.
Chemical hazard	Inherent property of an agent or situation having the potential to cause adverse effects when an organism, system, or (sub)population is exposed to that agent
Chemical risk	The probability of an adverse effect in an organism, system, or (sub)population caused under specified circumstances by exposure to an agent.
Circular economy	An economic system based on the reuse and regeneration of materials or products, especially as a means of continuing production in a sustainable or environmentally friendly way.
Hazardous waste	Waste prescribed by the *Hazardous Waste (Regulation of Exports and Imports) Act* 1989, where has any of the characteristics mentioned in Annex III to the Basel Convention, including: explosive; flammable liquids/solids; poisonous; toxic; ecotoxic; infectious substances.
Leachable components	Components that can migrate from a contact or carrier material into the environment.
Limit of detection	The lowest concentration of an analyte that, in a given matrix and with a specific method, has a 99% probability of being identified, qualitatively or quantitatively measured, and reported to be greater than zero.
Limit of quantitation	The concentration of analyte in a specific matrix for which the probability of producing analytical values above the method detection limit is 99 percent. It is the smallest amount that can be reliably identified and quantified by the method.
Limit of reporting	The lowest concentration of a chemical that can be determined with acceptable precision and accuracy under the stated conditions of a test. It is the practical limit of quantitation at or above the LOQ.
Relative percent difference	A statistic used to evaluate and normalise the difference between two measurements.

Abbreviations

Abbreviation	Definition
DCCEEW	Department of Climate Change, Energy, the Environment and Water
6PPD (-Q)	*N*-(1,3-dimethylbutyl)-*N*'-phenyl-*p*-phenylenediamine (-quinone)
ASLP	Australian Standard Leaching Procedure
ASU	CSIRO's Analytical Services Unit
BDE	Polybrominated diphenyl ether
BPA	Bisphenol A

Abbreviation	Definition
CAS RN	Chemical Abstracts Service Registry Number
CSIRO	Commonwealth Scientific and Industrial Research Organisation
CV	Coefficient of variation
DEECA	Department of Energy, Environment and Climate Action (Victoria)
DCM	Dichloromethane
DEHP	Bis(2-ethylhexyl) phthalate
DPG	Diphenyl guanidine
EC	Electrical conductivity
EOL	End of life
ESI	H-electrospray ionisation
GC-MS	Gas chromatography-mass spectrometry
HDPE	High density polyethylene
HMMM	Hexa(methoxymethyl)-melamine
HPLC	High-performance liquid chromatography
HRAMS	High-resolution accurate-mass mass spectrometer
IC	Ion chromatography
ICP-MS	Inductively coupled plasma-mass spectrometry
ICP-OES	Inductively coupled plasma-optical emission spectroscopy
IP3	Impact Priority 3
L/A ratio	Liquid-to-surface area ratio
L/S ratio	Liquid-to-solid ratio
LC	Liquid chromatography
LC-MS/MS	Liquid chromatography-mass spectrometry/mass spectrometry
LEAF	Leaching Environmental Assessment Framework
LIB	Lithium ion battery
LOR	Limit of reporting
MIBK	4-Methyl-2-pentanone
NATA	National Association of Testing Authorities
NEMP	National Environmental Management Plan
NESP	National Environmental Science Program
NMI	National Measurement Institute
PAH	Polyaromatic hydrocarbons
PCB	Printed circuit board; in the context of measured analytes, PCB will also denote ‘polychlorinated biphenyl’.
PFAS	per- and poly-fluoroalkyl substances
POP	Persistent organic pollutant
PP	Polypropylene
QA/QC	Quality Assurance/Quality Control
RP	Research Plan
RPD	Relative Percent Difference
RRS	Recycled Rubber Surfacing
SCaW	Sustainable Communities and Waste
SPE	Solid Phase Extraction
TOPA	Total oxidisable precursor assay
TPH	Total petroleum hydrocarbons
TRH	Total recoverable hydrocarbons

Abbreviation	Definition
TSA	Tyre Stewardship Australia
UHPLC	Ultra high-performance liquid chromatography
US EPA	United States Environmental Protection Agency

Contents

1. Introduction

The risk of chemicals (including currently unknown chemicals) in our waste streams are poorly defined. This key information gap inhibits our ability to safely move toward achieving national and state policy action targets to divert materials from landfill and accelerate their reuse. The presence of chemicals of concern in waste materials can impact their recyclability and safe reuse. As we move towards resource recovery and a circular economy, we need to ensure material reuse is safe and risks associated with chemicals of concern in waste are minimised for human, environmental and social well-being.

Through co-design with the Department of Climate Change, Energy, the Environment and Water (the Department), researchers from the National Environmental Science Program (NESP) Sustainable Communities and Waste (SCaW) Hub in Impact Priority 3 (IP3) identified three key themes for prioritisation of research:

1. What's in our waste? - understanding the chemicals in current and emerging wastes;
2. What's the risk profile of chemicals in our wastes? - de-risking the future through safe waste reuse and resource recovery; and
3. How do we better inform stakeholders of potential risks? - enhancing information flows and assessment for improved outcomes and governance for hazardous wastes.

Underlying these three key themes of research are critical data gaps on the composition/mass of chemicals in our wastes, their potential release to the environment and the safe reuse potential of our waste streams. These are recurring issues for risk-based decision making, regarding the management and treatment of wastes, including the safe reuse of recovered resources.

The work completed through Research Plan 2 (RP2; 2022) along with work to be conducted in forward years, aims to build national capability, and generate quantitative data and methodological guides that can be used for evidence-based risk management of chemicals identified in our wastes and in repurposed materials. RP2 has started to build a knowledge platform for the chemical composition of key waste streams and associated concentrations. RP3 (2023-2025) will identify the leachable components from these waste streams, and their behaviour under field or reprocessing conditions. Information sharing and hazardous waste governance will be enabled through improved baseline compositional and leachability data.

Given the short 9-month timeframe for research in RP2, aspects of the work have been planned to parallel and dovetail with those in RP3. Together, RP2 and RP3 will adopt a tiered analytical screening approach, whereby broad and systematic screening of compounds across targeted waste samples will be undertaken to generate reliable and re-usable analytical methodologies. RP2 has generated preliminary information regarding the chemical composition of key waste streams, including known chemicals and other components that may trigger further investigation based on preliminary risk assessments. This annual report summarises the research activities associated with RP2.

In addition, through a co-design process with the Department, the following has been produced in RP2:

– A draft leaching methodology for application in RP3;
– A preliminary guidance document for the robust and relevant sampling of complex waste streams;

– A data management strategy with data reporting template that meets the requirements of research users; and,
– Collaborative relationships within and outside the SCaW Hub with key research partners.

1.1 Background

During RP1 (2021-2022), a co-design process was undertaken with IP3 researchers and the Department, other regulatory agencies, and industry partners to determine key hazardous waste research priorities, and to develop a multi-year research agenda for the NESP SCaW Hub IP3, Hazardous Waste, Substances and Pollutants. In this consultation process, end of life (EOL) tyres and electronic waste (e-waste) were identified as the key wastes initially requiring characterisation of chemical composition. The findings of the RP1 co-design process are detailed in a summary report presented to the SCaW Hub in early 2022 [1].

EOL tyres and e-wastes are problematic wastes, with the bulk of wastes ending up in landfill or, historically, exported from Australia for treatment, recovery, or disposal. Recent Australian waste export bans and import bans by some of Australia's key waste management partners (e.g., China and the National Sword Policy banning the importation of recyclable materials) have resulted in significant environmental, economic and policy drivers to ensure that we manage, recycle and reuse wastes domestically [2, 3]. There are reportedly significant arisings of both e-waste and EOL tyres in urban, remote, and regional settings [4, 5, 6], with EOL tyres particularly linked to heavy industry and transport in regional and remote areas of Australia. Our Federal and State regulatory bodies share a consensus in identifying these waste streams as significant and problematic in Australia.

With the introduction of strong resource recovery targets and a push towards increasing the content of recycled materials, waste derived materials are increasingly being reused in new materials (e.g., tyre materials in road base, playground surfaces, tiling, or bunding). Some of these wastes can contain chemicals of concern (e.g., heavy metals like lead, cadmium and mercury, bisphenol A (BPA), per- and poly-fluoroalkyl substances (PFAS), *N*-(1,3-dimethylbutyl)-*N*'-phenyl-*p*-phenylenediamine quinone (6PPD-quinone; 6PPD-Q), polybrominated diphenyl ethers (PBDE), and other flame retardants) that have been shown to impact human and ecosystem health [7, 8, 9]. The fate of chemicals associated with EOL tyres and e-wastes during management, handling, processing and reuse of these wastes is not widely characterised. In addition, there is little to no data on the impact on Australia's unique biodiversity and ecosystems directly attributable to chemicals contained in EOL tyres and e-wastes. The lack of relevant and robust waste data limits risk-based decisions regarding the safe recovery and reuse of resources obtained from these and many other wastes [10]. Similarly, representative, and robust sampling guidelines for wastes, such as e-waste and EOL tyres, do not exist. Without accurate, quantitative, statistically robust data about what chemicals are in our waste, decisions regarding e-waste and waste tyre-derived materials and their safe reuse will continue to be hindered [11].

1.2 Project objectives for Research Plan 2

Using EOL tyres and e-wastes as our initial target waste streams (case studies), the key objectives for RP2 were:

1. To develop a robust sampling design and strategy for sampling Australian tyre and e-waste streams

A robust sampling strategy for EOL tyres and e-waste is critical to ensure confidence in risk and hazard assessments related to the safe reuse of wastes and recovered resources. For example, the volume/mass of subsamples recovered, frequency of subsampling, and considerations of strategies for sampling from waste piles can impact the quality and reliability of analytical data generated. Non representative samples may provide inaccurate information regarding thresholds or trigger limits and skew risk assessments for identified chemicals, or even fail to identify risks associated with chemicals.

In RP2, the IP3 research team and the Department co-designed a preliminary and transferrable guidance document using EOL tyres as a case study that outlines the iterative principles of sampling plan design for complex waste materials.

2. To build current and relevant quantitative analytical datasets for the composition, detectable limits, and concentrations of chemicals in Australian tyre and e-waste streams

To determine 'what's in our waste' and define hazards related to the chemicals which they may contain, reliable characterisation of EOL tyres and e-wastes and recovered waste-derived materials is required.

In RP2, concurrent modification and development of analytical methods to best determine the chemical composition of these wastes were conducted using analytical capability at CSIRO and Curtin University and associated commercial laboratories. Preliminary qualitative and quantitative characterisation of chemicals associated with a commercially available recycled rubber product and e-wastes were conducted. A data reporting tool was developed by the Department for the data generated in this project to be reported in a findable, accessible, interoperable, and re-usable (FAIR) data format.

3. To develop a methodology to assess leachability and potential availability of chemicals from tyre and e-wastes and associated re-purposed materials

In RP2, a draft methodology for assessing the leachable components in EOL tyres and recycled rubber products was developed by the IP3 research team, with input and feedback from the Department. The document outlines the preliminary experimental plan for assessment of leachable chemicals recycled rubber products and e-waste materials using standard and non-standard leaching and will allow further characterisation of these materials and foundation data for the development of ecotoxicology assessments in forward years of IP3 research.

2. Progress for Research Plan 2

Table 1 outlines the progress of RP2 with respect to defined deliverables identified during the proposal stage.

Table 1 Progress update for RP2 with respect to milestones.

Milestones	Due date	Comments
Milestone 1 – Signing of contract	1 Jul 2022	This contract date was delayed by 3 months, and this impacted the delivery of milestones and research objectives.
Milestone 2 – Scopes refined to agree type and locations of e-waste and tyre wastes.	30 Jul 2022, or 4 weeks/1 months after RP2 contract agreement	This was completed in July 2022, and where appropriate or permitted by the participating organisations, approval was sought to commence work prior to contract finalisation.
Milestone 3 – Analytical methodologies outlined for evaluation	30 Jul 2022 or 1 month after contract signing	This was completed in July 2022 through co-design between CSIRO and Curtin University analytical laboratories, with feedback from research users at the Department.
Milestone 4 – Sampling strategy for waste types drafted	31 Aug 2022 or 2 months after contract signing	A draft sampling guidance for complex waste characterisation using end of life tyres as a case study was prepared in January 2023. The draft document was provided to research users at the Department for comment in February 2023.
Milestone 5 – Circulation of draft priorities to include within RP3 – leaching and availability studies.	1 Aug 2022 depending on date of contract signing	This was completed in August 2022. As at February 9 2023, we are awaiting approval to commence RP3.
Milestone 6 – Analytical update for characterisation of chemicals in wastes	1 Oct 2022 or 3 months after contract signing	Samples were obtained to commence analytical work and to fast track method development and sampling guidance material. A preliminary analytical update was provided on 25th October 2022, and a fuller analysis was prepared and submitted to research users at the Department on 14 February 2023. There have been delays associated with securing additional samples from waste management and recycling companies.
Milestone 7 – Methodology for determining total leachable components	1 Oct 2022 or 3 months after contract signing	A draft methodology for determining total leachable components in waste samples for use in RP3 and beyond was prepared and sent to research users at the Department for comment on 14 February 2023.
Anticipated RP3 commencement (leachability and bioavailability)	Jan 2023	RP3 was approved in principle by the SCaW Hub, but contracts have not yet been finalised (as at 10 March 2023).
Milestone 8 – Draft report outlining approach to waste sampling, characterisation, and reporting. Feedback from co-design team and the Department	3 Feb 2023 (9 weeks prior to final report)	This report outlines the approach to waste sampling, characterisation, and reporting. Also included in feedback from the co-design team and research users at the Department. This report was sent to the Department for initial feedback on 7 March 2023.
Milestone 9 – Final RP2 report.	30 Apr 2023	To be completed considering feedback from Hub, researchers, and research users.

3. Research Plan 2 – Progress Report

3.1 Development of Sampling Guidance for complex waste streams

Through a review of relevant general waste sampling, contaminated sites and specific EOL tyre sampling guidance [12-20], a 5-point, iterative sampling plan design framework has been proposed, with the view of providing transferrable sample plan design advice across multiple complex waste streams and waste derived materials. The preliminary sampling guidance was submitted in draft form to the Department on 14 February and 9 March 2023. Feedback was received from the Department on 24 February and 2 May 2023 and is currently in revision.

Figure 1 Principles of sampling plan design for complex waste materials.The sampling plan design framework is illustrated in Figure 1, and described briefly here.

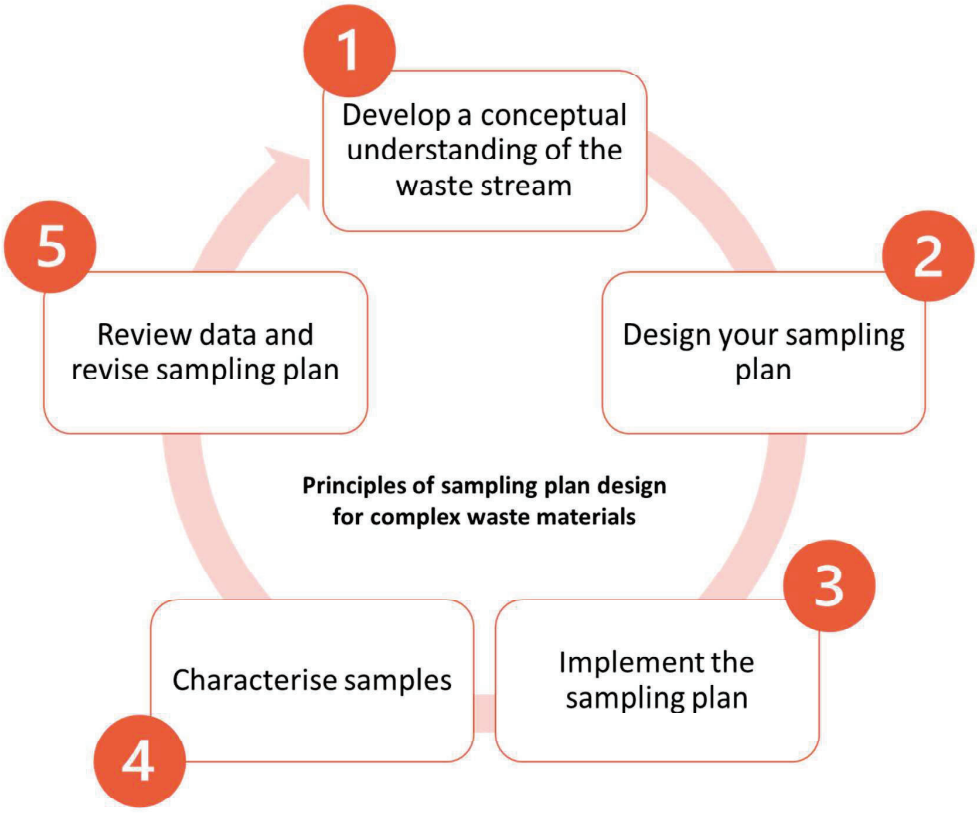

Figure 1 Principles of sampling plan design for complex waste materials.

1. Develop a conceptual understanding of the waste stream

A conceptual understanding of the target waste stream and processes involved in waste handling and recycling is a critical step in sampling plan design, which includes defining the purpose of the sampling campaign and understanding how and why the data generated from collected samples will be used, who the data users will be and how the data generated will achieve the purpose of the sampling plan.

2. Design your sampling plan

A preliminary sampling plan for waste or waste derived materials can be developed by combining the established conceptual understanding of the waste material, a review of existing or acceptable guidelines and standards related to sampling of similar or like materials, where available, or an understanding of gaps in knowledge, and an assessment (using available literature and information) or judgement (when literature and information is limited) of the likely types of chemicals present in the waste.

In future iterations of sampling plans that go beyond initial characterisation of waste materials, a sampling plan must consider the application of statistics to design appropriate sampling strategies that can generate information with quantitative insights related to the materials being sampled.

3. Implement the sampling plan

Following the designed sampling methodology, samples can be collected and appropriately stored prior to analysis. At the same time, metadata related to the sampling event should also be recorded.

4. Characterisation of samples

Samples should be characterised by accredited analytical laboratories, considering instruction guidelines related to consistent data reporting for efficient data analysis and review.

5. Review data and revise sampling plan

After samples have been characterised, the data generated should be analysed, interpreted, and reported as required. The sampling plan can be iteratively modified based on this review process to ensure that sampling is undertaken in a manner that supports the goal of the sampling plan.

3.2 Characterisation of recycled rubber and e-waste samples

3.2.1 Overview

Initial chemical characterisation of a commercial recycled rubber product and two e-waste samples was undertaken to address the following specific objectives:

– To understand chemicals that are present in a recycled rubber product and e-waste;

– To guide the development of sampling guidance and characterisation, leachability and ecotoxicology methodology using recycled rubber and e-waste samples as case studies; and,

– To provide a test case for handling and reporting of data that is consistent with data reporting standards described in the National Principles for Environmental Information and can be readily used by the Department.

This section describes materials and methods used for the characterisation of samples, and a preliminary discussion of results obtained from recycled rubber products and e-waste samples.

The data generated from these analyses were used as a test case to build and iteratively develop a data management template. Key achievements and challenges associated with the analysis of these materials and the implications for complex waste characterisation are also discussed.

3.2.2 Data management and limitations

Data for recycled rubber products and e-waste samples were recorded in version 1 of the data reporting tool developed and discussed in Section 6.2. The data set identifier is *IP3_DS3-Understanding chemicals in our wastes and recovered resources (Annual Progress Report, 2022)*. Further information related to samples, methods, and other related data can be found in this workbook.

The data in this workbook is limited to a small number of samples, with limited replicates available. The full datasets are generated from multiple sources and some manual data handling and compilation of individual datasets has been completed. In some instances, information and data related to methods, standards and QA/QC procedures from external laboratories has not been made available for reporting. Interpretations and use of data in this workbook is not verifiable or supported by authors of the data. The NESP SCAW Hub and its partners accept no liability for use of data in this workbook, and all data is held in confidence until all final approvals for public release are provided.

3.2.3 Materials and methods

3.2.3.1 Samples and sample preparation

Three samples were analysed for preliminary characterisation of chemicals that may be associated with EOL tyres and e-wastes. A summary of samples provided for analysis, including relevant sample preparation information is shown in Table 2.

Table 2 Samples analysed for preliminary characterisation of chemicals that may be associated with EOL tyres and e-wastes.

Sample ID	Sample Description	Source	Sample Preparation	Citation
RRS	A commercially available recycled rubber product used for landscaping	Purchased from a hardware store	Where necessary, the recycled rubber product was cryogenically milled using a Rocklabs Benchtop Ring Mill. Samples were placed in the ring mill container and cooled by pouring liquid nitrogen into the chamber. The samples were cooled for 5 minutes or until boiling had subsided. The frozen samples were milled for 2 minutes.	n/a
PCBW	Pulverised printed circuit boards (PCB)	CSIRO Sample Repository	None required	21
LIBW	Pulverised cathodes from lithium ion batteries (LIB)	CSIRO Sample Repository	None required	22

Sample containers used for sample handling were dependent on the analysis to be undertaken. For both sample types, polypropylene (PP) containers were used to handle samples for inorganic analyses, whilst glass containers were used for samples for organic analysis. For PFAS analysis, high density polyethylene (HDPE) containers were used to prevent mass transfer of compounds to container walls and minimise error in analysis.

3.2.3.2 Analytical methods

A summary of the various analytical regimes for characterisation of samples is provided in Table 3. Standard analytical suites were undertaken by external laboratories who were NATA-accredited (where possible), with established methodologies in place for screening of some chemicals. However, some engagement with external laboratories was still required to ensure samples were handled appropriately prior to analysis and to receive sufficient information on the used methods and results.

The analytes were selected based on the information available related to chemicals that could be present in the selected waste types (EOL tyres as an e.g., Table 4), and the availability of methods for analysis. A summary of relevant Chemical Abstracts Service Registry Numbers (CAS RN) for analytes is provided in Appendix 1.

Table 3 A summary of analytical regimes for characterisation of recycled rubber product and e-waste samples.

Class	Analyte or analyte group	Number of compounds analysed	Sample types		Laboratory	Method Code#
			RRS	Electronic waste (PCBW and LIBW)		
Inorganic	Trace Elements	18	Y	Y	CSIRO	CS-ICPMAD
Inorganic	Major Elements	5	Y	Y	CSIRO	CS-ICPOAD
Inorganic	Major Anions	5	Y	Y	CSIRO	CS-IC
Inorganic	Other (pH, EC, %C)	-	Y	Y	CSIRO	CS-pH CS-EC CS-TC
Organic	Amines Nitroaromatics & Nitrosamines	12	Y	Y	NMI	NMI 1122 Screen
Organic	Brominated-diphenyl Ethers (BDEs)	36*	N	Y	NMI	AUTL_MET_003
Organic	Ethers	5	Y	Y	NMI	NMI 1120 Screen
Organic	Halogenated Aliphatic Hydrocarbons	32	Y	Y	NMI	NMI 1120 Screen
Organic	Halogenated Aromatic Hydrocarbons	12	Y	Y	NMI	NMI 1122 Screen
Organic	Monocyclic Aromatic Hydrocarbons	14*	Y	Y	NMI	NMI 1122 Screen
Organic	NEPM Total Recoverable Hydrocarbons (TRH)	6	Y	N	NMI	NMI 1120 Screen
Organic	Organochlorine Pesticides	16	Y	Y	NMI	NMI 1122 Screen
Organic	Organophosphate Pesticides	6	Y	Y	NMI	NMI 1122 Screen
Organic	Other Organic Compounds	7	Y	Y	NMI	NMI 1122 Screen
Organic	Oxygenated Compounds	6	Y	Y	NMI	NMI 1120 Screen
Organic	Per- and polyfluoroalkyl substances (PFAS)	30 (Eurofins) 38 (Curtin)	Y	Y	Eurofins + Curtin (method under development)	PFAS (CWQRG) PFAS (Eurofins)
Organic	Phenols	13*	Y	Y	NMI	NMI 1122 Screen
Organic	Phthalates	6	Y	Y	NMI	NMI 1122 Screen

Class	Analyte or analyte group	Number of compounds analysed	Sample types		Laboratory	Method Code#
			RRS	Electronic waste (PCBW and LIBW)		
Organic	Polychlorinated biphenyl	22*	N	Y	NMI	NMI 1122 Screen
Organic	Polycyclic Aromatic Hydrocarbons	16*	Y	Y	NMI	NMI 1122 Screen
Organic	Triazoles	2	Y	N	Eurofins	EF-TRIA
Organic	Total Recoverable Hydrocarbons (formerly TPH)	4	Y	Y	NMI	NMI 1120 Screen
Organic	Trihalomethanes	4	Y	Y	NMI	NMI 1120 Screen
Organic	Tyre chemicals‡	2	Y	N	CSIRO + Eurofins	EF-TYRE CS-TYRE1 CS-TYRE2

*Discrete and mixtures; ‡ refer to Appendix 1 for details

Table 4 Types and classes of chemicals predicted for EOL tyres and rubber materials.

Types and classes of chemicals*	Reference
Polycyclic aromatic hydrocarbons (PAHs)	23
Phthalates	7
Benzotriazoles and benzothiazoles	23
Bisphenol A/S/F	7
6PPD (6PPD-quinone) N,N'-Diphenylguanidine (DPG) Hexamethoxymethyl-melamine	7, 24, 25
Inorganics (e.g., Pb, Zn, Cr, Cd, Co)	7

Below are brief descriptions of the methods used to quantify the different groups of chemicals. These, along with the relevant method codes, are also provided in the data sheet attachment.

Inorganic analyses

Analysis of different elements (i.e., metals, non-metals, metalloids) and anions were conducted by the Analytical Services Unit (ASU) (CSIRO Waite, South Australia).

– For analysis of different metals, non-metals, and metalloids, samples were digested in reverse aqua regia (3:1, nitric acid: hydrochloric acid). Extracts were passed through a 0.45 µm cellulose filter then quantified by inductively coupled plasma-optical emission spectroscopy (ICP-OES) and inductively coupled plasma-mass spectrometry (ICP-MS), using an Agilent 5100 ICP-OES and ICP-MS systems. (Method codes: CS-ICPMAD, CS-ICPOAD)

– Analysis of anions were conducted by ion chromatography (IC) on 1:5 water extracts using a Shimadzu module IC system.(Method code CS-IC)

– Other analyses included pH and electrical conductivity (EC) measurements. (Method codes: CS-pH, CS-EC)

Organic analyses

Total carbon content of the samples was measured by the ASU (CSIRO, Method code: CS-TC), where 0.1 g of sample was processed by a combustion analyser (LECO Corporation). Recycled rubber product and e-waste samples were processed for analysis of different volatile and semi-volatile organic compounds at the National Measurement Institute (NMI, North Ryde, NSW). Samples were extracted using a 50:50 mixture of dichloromethane and acetone, with the extract

analysed by gas chromatography-mass spectrometry (GC-MS). The extraction and analytical procedure were based on US EPA Method 8270 (Method codes: NMI 1120 and NMI 1122 Screen).

Analysis of relevant tyre chemicals was conducted by Eurofins (Brisbane, Queensland). Their analyses were focused on triazoles, as well as 6PPD-Q and hexa(methoxymethyl)-melamine (HMMM). The triazoles were run with an in-house method, and ultrapure water was used as the extraction solvent (Method code: EF-TRIA), whilst 6PPD-Q and HMMM were extracted from the tyre crumb using dichloromethane and acetonitrile (Method code: EF-TYRE).

Quantification of 6PPD-Q was undertaken at CSIRO (Waite, South Australia). Recycled rubber product samples were extracted twice with methanol, once by a 50:50 mixture of acetone and hexane solvent, followed by liquid chromatography-tandem mass spectrometry (LC-MS/MS) analysis. (Method code: CS-TYRE1) To enable direct comparison with results provided by Eurofins, the same solvent composition (dichloromethane and acetonitrile) was also used for repeat extraction of samples at CSIRO. Extracts were also analysed by LC-MS/MS. (Method code: CS-TYRE2)

Samples analysed at CSIRO were quantified based on at least a 5-point calibration curve with standards (0 to 100 µg/L) prepared in 100 % methanol, as per samples. Only curves with regression coefficients (R^2) above 0.975 were considered acceptable for quantitation. Samples were quantified comparing the response of analytes in samples with the response in a calibration curve. For 6PPD-Q, which had an isotopically labelled standard available, quantitation was based on an internal standard calibration where relative response of the analyte and stable isotope analogue was compared in samples and standard solutions.

Preliminary (qualitative) PFAS identification of 38 PFAS in the non-milled recycled rubber product sample was undertaken by Curtin University (Perth, Western Australia) (Method code: PFAS (CWQRG)). Samples were extracted twice with methanol , followed by two sequential extractions with 1:1 hexane:acetone , and subjected to solid-phase extraction. PFAS were detected using ultra-high-performance liquid chromatography-high-resolution accurate-mass mass spectrometry (UHPLC-HRAM MS). PFAS analytical standards (n=36) and deuterated PFAS analytical standards (n=24) were purchased from Wellington Laboratories, Canada. Trifluoroacetic acid and perfluoropropionic acid were purchased from Sigma Aldrich, Australia. PFAS contamination was minimised by a) installation of a Thermo Scientific™ PFC-free kit in the UPLC system; b) installation of isolator column after the LC pump and prior to the injection valve to offset any contaminants from the LC pump, autosampler, degasser and mobile phases; c) use of HDPE vials and bottles, rather than glass; d) vials, tubes, pipette tips disposed of after use, rather than cleaned and re-used; e) workbench cleaned with methanol before sampling and extraction; f) use of LC-grade solvents including water; and, g) analysis of full method blanks and solvent blanks.

PFAS identification and quantitation in the milled recycled rubber product and e-waste samples was undertaken at Eurofins (Brisbane, Queensland) using LC-MS/MS (Method code: PFAS (Eurofins)). The samples were transported in HDPE containers (without PTFE-lined caps) and spiked with isotopically labelled PFAS standards, extracted into basic methanol, and cleaned up by carbon and SPE cartridges following US EPA method 1633 (3rd revision), before analysis for 30 PFAS [26]. Method blanks were performed on laboratory certified clean sands and met pass limits (<LOR) for all PFAS analytes. The cleaned-up extracts were also dried and dissolved in purified water in an HDPE bottle for PFAS total oxidisable precursor assay (TOPA) (Method code: TOPA (Eurofins)). This aqueous sample was subjected to hydroxyl radical-based oxidation, followed by clean-up and elution in an adaptation of the method of Houtz and Sedlak [27, 28]. TOPA sample solutions were then analysed for 30 PFAS.

3.2.3.3 Sample variability (recycled rubber product only)

The potential variability of the samples obtained from the recycled rubber product was investigated by collecting seven (7) subsamples from the bulk sample and sending them for elemental analysis. The effect of particle size/ grinding on the reported analyte concentrations was investigated for the crumbed tyre rubber sample. To determine the potential impact of particle size on analysis,

samples were flash frozen then ground using a coffee grinder. The comparison of particle size was conducted on the analysis of 6PPD-Q. Given the amount of sample typically extracted is <0.5 g, grinding also further homogenised the sample and enabled collection of subsamples that were representative of the bulk sample.

3.2.3.4 Quality assurance and control

To ensure quality of the data obtained from the various analyses, Quality Assurance and Control (QA/QC) measures were followed and a summary is provided in Table 5. For each QA/QC measure, acceptance limits and corrective actions to achieve the acceptance limits are specified.

Table 5 Summary of internal QA/QC applied at CSIRO and Curtin laboratories

	QA/QC Measures	Description	Acceptance Limit*	Corrective Action
Sample Handling	Storage	Samples stored at 4 °C (or at an appropriate temperature) when not in use	Temperature of storage room needs to be maintained within 1-4 °C	Deviation from these temperatures triggers alert where samples are transferred to appropriate temperature storage
Analytical	Replicates	Minimum of 2 extractions, including blanks and spikes	≤ 30-50 % Relative percent difference or Coefficient of variation (CV) – except for blanks where results are < Reporting limit	Investigate; Repeat until requirement is achieved
	Method Blanks	Reagent only to test for contamination	< Reporting limit	Investigate; Repeat until requirement is achieved
	Fortified Blanks	Spiked blank	50-150 % Recovery of spiked reagents	Investigate; Repeat until requirement is achieved
	Fortified Samples	Spiked sample to establish recovery	50-150 % Recovery	Investigate; Repeat until requirement is achieved
	Isotope Recoveries (where available)	Isotope spiked to all samples to estimate recovery	50-150 % Recovery	Investigate; Repeat until requirement is achieved

* Listed here are general QA/QC guidance. Acceptance limits and QA/QC methodology are laboratory specific. Analysis by external laboratories may have wider, or narrower acceptance ranges than reported here depending on the methods used for analysis, and these should be reported with data generated from any study as a minimum requirement. Where available, this has been reported in the data set associated with this annual report (*IP3_DS3*). However, it should be noted that in some cases this information is not available for all compounds.

Where external laboratories were engaged to complete analysis, a summary of QA/QC methodology was requested. Where provided, this information is included associated with reportable data in the data reporting template (under the sheet titled “Batch” in *IP3_DS3*; Current set of data covers BatchID B001 to B007).

In addition, an interlaboratory comparison between analysis of 6PPD-Q undertaken at CSIRO and Eurofins was also performed using samples from the recycled rubber product.

3.2.4 Results and discussion

When visually inspected, the recycled rubber product was granular (particle size ranging from 1-4 mm), and was predominantly composed of black coloured particles, interspersed with a lower proportion of grey particles (Figure 2).

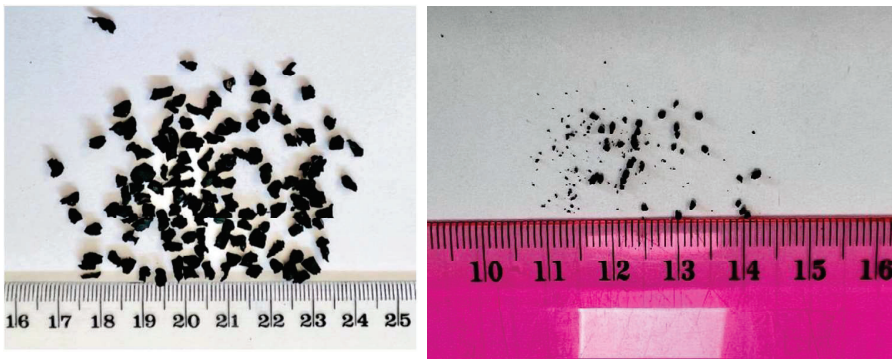

Figure 2 Recycled rubber product in coarse (A) and ground (B) forms analysed for chemical characterisation.

The e-waste samples were visually characterised as exceptionally fine powders, with particle size <500 µm. The PCBs were grey in colour (Figure 3A), and the LIBs were black in colour (Figure 3B).

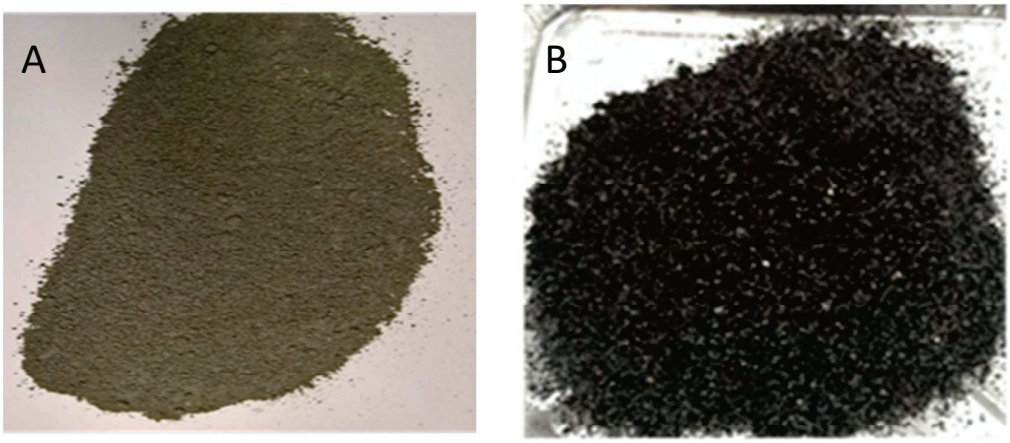

Figure 3 Pulverised printed circuit boards (A) and lithium ion battery (B) materials sourced from CSIRO's sample repository for chemical characterisation of e-waste materials.

A total of 253 discrete chemicals and 26 mixtures (e.g., total C, total PBDEs) were analysed for the recycled rubber and e-waste samples (Table 6; Table 7). The reported data for the recycled rubber samples consisted of 82 % organic chemicals and mixtures, while the inorganic components made up the remaining 18 %. Similarly, for the e-waste samples, the reported data consisted of 91 % organic chemicals and mixtures, while the inorganic components made up the remaining 9 %. For a full list of analysed chemicals, including those that were detected below LOR or MDLs, please refer to the data in the associated data set, *IP3_DS3*.

3.2.4.1 Characterisation of recycled rubber product

A summary of inorganic and organic chemicals detected in samples of recycled rubber product are shown in Table 6. The total carbon content (79.6 %) is consistent with the typically reported carbon content of tyres (74-76 %) [29]. Total recoverable hydrocarbons (TRH) were approximately 1.7 % w/w for C10-C40 fractions, which indicated that a fraction of the total carbon measured was derived from hydrocarbons. Sulfur content (1.2 % w/w) was high which was expected and commonly reported (~1.6 % w/w) due to its use as a vulcanisation agent for tyres [30]. Except for S and Zn, all the other elements found in the recycled rubber product were ≤ 0.4% w/w.

Table 6 Concentrations of different inorganic and organic chemicals detected in samples of recycled rubber product (sub-sample identifier, RRS1TP0922). Analytes that were not detected are not noted in this table.

Inorganic	Concentration (unit)		Organic	Concentration (unit)	
Al	391 ± 169	mg/kg	Fluoranthene	2.2	mg/kg
As	0.38 ± 0.17	mg/kg	Phenanthrene	1.6	mg/kg
Ca	691 ± 1133	mg/kg	Pyrene	5.7	mg/kg
Cd	0.60 ± 0.29	mg/kg	Phenol	1.0	mg/kg
Co	132 ± 78	mg/kg	Aniline	7.8	mg/kg
Cr	2.04 ± 0.34	mg/kg	*N*-Nitrosodi-n-propylamine	2.6	mg/kg
Cu	31 ± 6	mg/kg	4-Methyl-2-pentanone (MIBK)	17	mg/kg
Fe	183 ± 64	mg/kg	Bis(2-ethylhexyl) phthalate (DEHP)	3.2	mg/kg
K	132[@]	mg/kg	6PPD-Q	13,509 ± 1771[#]	µg/kg
Mg	73 ± 14	mg/kg	HMMM	7,100	µg/kg
Mn	4.43 ± 2.62	mg/kg	TRH C10 - C14	200	mg/kg
Mo	0.10 ± 0.03	mg/kg	TRH C15 - C28	7,000	mg/kg
Na	193 ± 36	mg/kg	TRH C29 - C36	6,500	mg/kg
Ni	2.44 ± 0.77	mg/kg	TRH>C10 - C16	270	mg/kg
P	112 ± 19	mg/kg	TRH>C10 - C16 less Naphthalene	270	mg/kg
Pb	21 ± 9	mg/kg	TRH>C16 - C34(F3)	13,000	mg/kg
S	12,729 ± 970	mg/kg	TRH>C34 - C40(F4)	3,400	mg/kg
Se	0.26 ± 0.06	mg/kg			
Sb	0.49 ± 0.19	mg/kg			
Sr	1.62 ± 0.99	mg/kg			
Zn	15,157 ± 2218	mg/kg			
Total C	80 ± 3	%			
Br^-	6.3 ± 0.6	mg/kg			
Cl^-	11 ± 3	mg/kg			
SO_4^{2-}	8.2 ± 0.3	mg/kg			
EC	45.2 ± 4.0	µS/cm			
pH	7.3 ± 0.2				

*This sample were not subjected to PBDE and PCB analyses.
Numbers are based on a single analytical sample unless otherwise indicated. Inorganic analysis is based on n=7 samples, shown as average ± standard deviation. [@]K was only detected in 1 out of 7 replicates. [#]6PPD-Q analysis is based on 3 separate analyses by CSIRO (2x) and Eurofins. Measurements from a 1:5 water shake are in orange (see Section 3.2.2.2).

The main findings relating to the chemical characterisation of the recycled rubber product samples were:

– The tyre additive HMMM (7 mg/kg) and the quinone derivative of the tyre additive 6PPD (6PPD-Q; 13 mg/kg) were quantified above their respective Limit of Reporting (LOR, 0.04 mg/kg) in the extracts prepared from the recycled rubber products. HMMM is used as a cross-linking agent, while 6PPD is used to protect the tyre against degradation by ozone. 6PPD is readily converted to its quinone derivative 6PPD-Q, and the relatively high concentrations of HMMM and 6PPD-Q in the recycled rubber product samples align well with other literature related to these materials [23, 31].
– Other chemicals of note in the recycled rubber product samples include the polycyclic aromatic hydrocarbons (PAHs) phenanthrene, fluoranthene and pyrene measured at low mg/kg concentrations [32].
– 4-Methyl-2-pentanone (or MIBK) was also detected (17 mg/kg) and may have been present as a precursor to produce 6PPD [33].
– Bis(2-ethylhexyl) phthalate (or DEHP) was found at 3 mg/kg. This class of chemical can be used for their plasticising properties in tyre rubber and have been found in different rubber materials [7, 32], but given their low detection in these materials, the source of the chemicals would need to be further investigated.
– Aniline (7.8 mg/kg) and *N*-nitrosodi-n-propylamine (2.6 mg/kg) were also measured above their respective LORs, but at low mg/kg concentrations [23, 34].
– In a preliminary analysis (method under development at Curtin University, so quantification and LOR not yet available), none of the targeted 38 PFAS compounds were detected in non-milled recycled rubber product.
– TOPA (LORs either 5 or 10 µg/kg) and analysis of 30 PFAS (LORs either 5 or 10 µg/kg) by Eurofins also did not detect PFAS or PFAS precursors in the milled recycled rubber product.
– All the organic chemicals present in the sample contributed to the total measured TRH fraction, which was around 1 % w/w of the sample weight (or 16 g/kg). This indicates that there are likely many other organic chemicals in the sample that were not quantified using the available analytical methods. Therefore, additional methods, such as HRAMS, would be required for a complete characterisation of the chemical content of the recycled rubber product samples.

3.2.4.2 Characterisation of e-waste samples

The chemicals identified in the pulverised LIB and PCB were consistent with e-waste streams which typically have a mix of metals, metalloids, glass, and plastics [29]. A summary of inorganic and organic chemicals (including flame retardants and other additives) detected in samples of PCBs and LIBs are shown in Table 7.

TRH were 0.04 and 0.08 % (w/w) in the LIB and PCB samples, respectively, from the C16-C40 fractions. Diethyl phthalate and DEHP were quantified in both LIB (3.6 and 110 mg/kg) and PCB (1.8 and 2.8 mg/kg) samples. Fluoranthene was the only PAH measured in the PCB samples, albeit close to its LOR (1 mg/kg). Phenol was also quantified in the PCB sample at 4.2 mg/kg. Phthalates are a common component of plastic materials where they are added as plasticisers or used as solvents in manufacturing processes, but given the low concentrations detected in this study, the source of these chemicals would need to be further investigated. .

A broad suite of BDE congeners was detected in both the LIB and PCB samples. Predominantly, BDE 209 was detected at 3.04 mg/kg and 2.25 mg/kg in the LIB and PCB samples, respectively. As BDEs are typically used in e-waste plastics for their flame retardant properties, it is unsurprising that these chemicals were detected in e-waste samples analysed in this project, but the concentration of these chemicals is lower than may be attributed to a functional chemical. Further investigation would be required to determine the source of these chemicals. The only relevant threshold limits for BDE are the health investigation level (HILs) developed by the National

Environmental Protection Council for site contamination [17]. The BDE HILs are limits for soil based on the potential exposure and toxicity to BDEs, are between 1 and 10 mg/kg for the total sum of measured BDEs [35], and the sum of BDEs found in both products is within this range. The HILs outlined in this document may not be broadly relevant for BDE detection in waste materials, and hence, further assessment of availability and toxicity of these compounds as they relate to waste materials is required.

Metals such as copper (Cu), cadmium (Cd), lead (Pb), nickel (Ni), and zinc (Zn), and metalloids such as antimony (Sb), are used to manufacture many electrical and electronic equipment items, but the concentrations of these vary depending on the type and properties required for the devices. Metals and other trace elements were typically elevated in both the LIB and PCB samples, albeit with different element profiles demonstrative of their functions. The concentrations of metals and other trace elements varied between the LIB and PCB samples, depending on the type and function of the devices. For example, Sb detected in PCBW (387 mg/kg) is likely a constituent of components conferring flame retarding properties, and the high concentration of cobalt (213,333 mg/kg) associated with LIBW, likely relates to the use of this metal in battery cathode materials. Other notable results for metals analysis include high concentrations of Cu, which is often used as a solid metal in foils and wires in the construction LIB (132,333 mg/kg) and PCBs (246,000 mg/kg), respectively. It should be noted that lithium (Li) was not analysed in this study as it was outside of the standard suite of metals for analysis. Previous characterisation studies have shown that the content of Li in the LIBW is 2.6 % (w/w) [22].

Two PFAS analytes were measured above the limit of reporting in the two e-waste samples. Perfluorobutanesulfonic acid (PFBS) was detected in the PCB sample (8.6 µg/kg) and perfluorooctanoic acid (PFOA) was detected in the LIB sample (470 µg/kg). TOPA indicated that there was an absence of oxidisable perfluoroalkyl acid (PFAA) precursors in these samples.

PFBS is known to be a component of photoacid generators [36], which are used in photolithography for integrated circuit manufacturing. The presence of PFBS in the powdered printed circuit board sample is also consistent with PFBS being detected in wastewater samples from three US electronics fabrication facilities, where PFBS was detected at locations that only contained wastewater from the photolithography step [37]. Interestingly, other PFAS (GenX (hexafluoropropylene oxide dimer acid, ammonium salt), PFBA, PFHxA, PFHpA, PFOA, PFNA and PFDA) were also detected at these locations, but the average mass concentration of PFBS was always higher than these other PFAS [37].

The presence of PFOA in the powdered LIB cathode is not surprising. PFOA is a processing aid in the polymerisation reaction to form poly(vinylidene fluoride) (PVDF) which is used as a binder in lithium ion battery cathodes [38] and PFOA has been found in environmental samples close to a PVDF production plant in Lyon, France [39]. PFOA is a Persistent Organic Pollutant (POP) listed on the Stockholm Convention. There is a specific exemption for its use in manufacture of PVDF to produce “industrial sealants capable of preventing leakage of VOCs and PM2.5 particulates [40]. Further review is needed to determine if its use in LIB cathodes fits into this purpose.

According to Australia’s PFAS National Environmental Management Plan Version 2 [41], the landfill acceptance criteria for total PFAS concentration in solid PFAS-contaminated materials has been capped at 50 mg/kg, based on the Stockholm Convention. The PFAS concentrations in the individual components of e-waste analysed in the current study are at least 2 orders of magnitude lower than the landfill acceptance criteria.

Table 7 Concentrations of different inorganic and organic chemicals detected in pulverised LIBW and pulverised PCBW samples. Analytes that were not detected are not noted in this table.

LIBW*						PCBW*								
Inorganic	Concentration		Organic	Concentration		Inorganic	Concentration		Organic	Concentration		Organic	Concentration	
Al	49,167 ± 351	mg/kg	BDE 183	1.1	µg/kg	Al	14,400 ± 1136	mg/kg	BDE 100	0.3	µg/kg	BDE 49	6.1	µg/kg
As	70.1 ± 4.5	mg/kg	BDE 184	0.2	µg/kg	As	19.3 ± 1.5	mg/kg	BDE 119	0.7	µg/kg	BDE 66	4.5	µg/kg
Ca	487 ± 15	mg/kg	BDE 196	3.4	µg/kg	B	2657 ± 107	mg/kg	BDE 138 + 166	0.9	µg/kg	BDE 71	1.8	µg/kg
Cd	533 ± 189	mg/kg	BDE 197	3.6	µg/kg	Ca	14,967 ± 153	mg/kg	BDE 139	0.6	µg/kg	BDE 77	0.7	µg/kg
Co	213,333 ± 9073	mg/kg	BDE 201	3.8	µg/kg	Co	66.6 ± 33.4	mg/kg	BDE 140	0.8	µg/kg	BDE 99	4.3	µg/kg
Cr	171 ± 42	mg/kg	BDE 203	5.3	µg/kg	Cr	33.2 ± 5.1	mg/kg	BDE 153	55.0	µg/kg	Fluoranthene	1.1	mg/kg
Cu	132,333 ± 577	mg/kg	BDE 206	90.0	µg/kg	Cu	246,000 ± 9644	mg/kg	BDE 154	6.1	µg/kg	PFBS	8.6	µg/kg
Fe	15,433 ± 1704	mg/kg	BDE 207	100	µg/kg	Fe	13,800 ± 3439	mg/kg	BDE 171	2.7	µg/kg	Phenol	4.2	mg/kg
K	2,717 ± 38	mg/kg	BDE 208	69.0	µg/kg	K	133 ± 2	mg/kg	BDE 180	19.0	µg/kg	Bis(2-ethylhexyl) phthalate	2.8	mg/kg
Mg	513 ± 11	mg/kg	BDE 209	3040	µg/kg	Mg	881 ± 18	mg/kg	BDE 183	690	µg/kg	Diethyl phthalate	1.8	mg/kg
Mn	9,953 ± 168	mg/kg	BDE 47	0.3	µg/kg	Mn	402 ± 8	mg/kg	BDE 184	3.0	µg/kg	TRH C15 - C28	594	mg/kg
Na	610 ± 9	mg/kg	BDE 49	0.1	µg/kg	Mo	23.9 ± 0.1	mg/kg	BDE 196	120	µg/kg	TRH C29 - C36	122	mg/kg
Ni	54,867 ± 777	mg/kg	BDE 99	0.1	µg/kg	Na	384 ± 9	mg/kg	BDE 197	250	µg/kg			
P	2,897 ± 45	mg/kg	Bis(2-ethylhexyl) phthalate	110	mg/kg	Ni	9,200 ± 677	mg/kg	BDE 201	29.0	µg/kg			
S	332 ± 16	mg/kg	Diethyl phthalate	3.6	mg/kg	P	628 ± 28	mg/kg	BDE 203	130	µg/kg			
Zn	1,060 ± 17	mg/kg	PFOA	470	µg/kg	Pb	1,363 ± 38	mg/kg	BDE 206	120	µg/kg			
E.C.	4,445 ± 142	µS/cm	TRH C15 - C28	240	mg/kg	S	721 ± 12	mg/kg	BDE 207	330	µg/kg			
pH	11.0 ± 0.1		TRH C29 - C36	140	mg/kg	Sb	387 ± 15	mg/kg	BDE 208	130	µg/kg			
						Zn	562 ± 11	mg/kg	BDE 209	2,250	µg/kg			
						E.C.	78.5 ± 3.1	µS/cm	BDE 28 + 33	5.7	µg/kg			
						pH	8.3 ± 0.1		BDE 47	5.6	µg/kg			

*These samples were not subjected to analysis of tyre-related chemicals; anions and total carbon results are pending.
Numbers are based on a single analysis unless otherwise indicated. Inorganic analysis is based on n=7 samples, shown as average ± standard deviation. Measurements from a 1:5 water shake are in orange

3.2.4.3 Other characteristics of samples obtained from recycled rubber product

Sample homogeneity was investigated for samples obtained from the recycled rubber product using elemental analysis performed on subsamples of materials (n=7). Results from analysis of these subsamples are in **Error! Reference source not found.**.

For the elemental analysis, overall variability (based on CV) for ICP-OES and ICP-MS analysis was ~40 %, although Ca (164 %), Mn (59 %) and Se (61 %) may have unduly influenced sample variability. Generally, a CV of >30 % is considered highly variable [42]. The overall variability suggested that the recycled rubber product was a reasonably homogeneous and well mixed sample, but the variability reported for some individual components detected in the waste as shown in Figure 4 (despite the apparent homogeneity of the sample) still highlighted that sample replicates were critical to overcome sample variability and that sample replicates are necessary for waste material analysis. A variability assessment is critical and should be completed for each sampling event for waste materials, regardless of sample frequency or analytical costs as it gives context analytical schedules chosen for characterisation purposes.

The effect of particle size/grinding on the reported analyte concentrations was investigated for the recycled rubber product sample. Reducing the particle size of the samples could potentially increase the surface area of the samples, which may facilitate extraction of the target analytes, but may also impact the overall availability of analytes because of size reduction. Table 8 Table 8 summarises the analysis of 6PPD-Q in coarsely crumbed and ground samples.

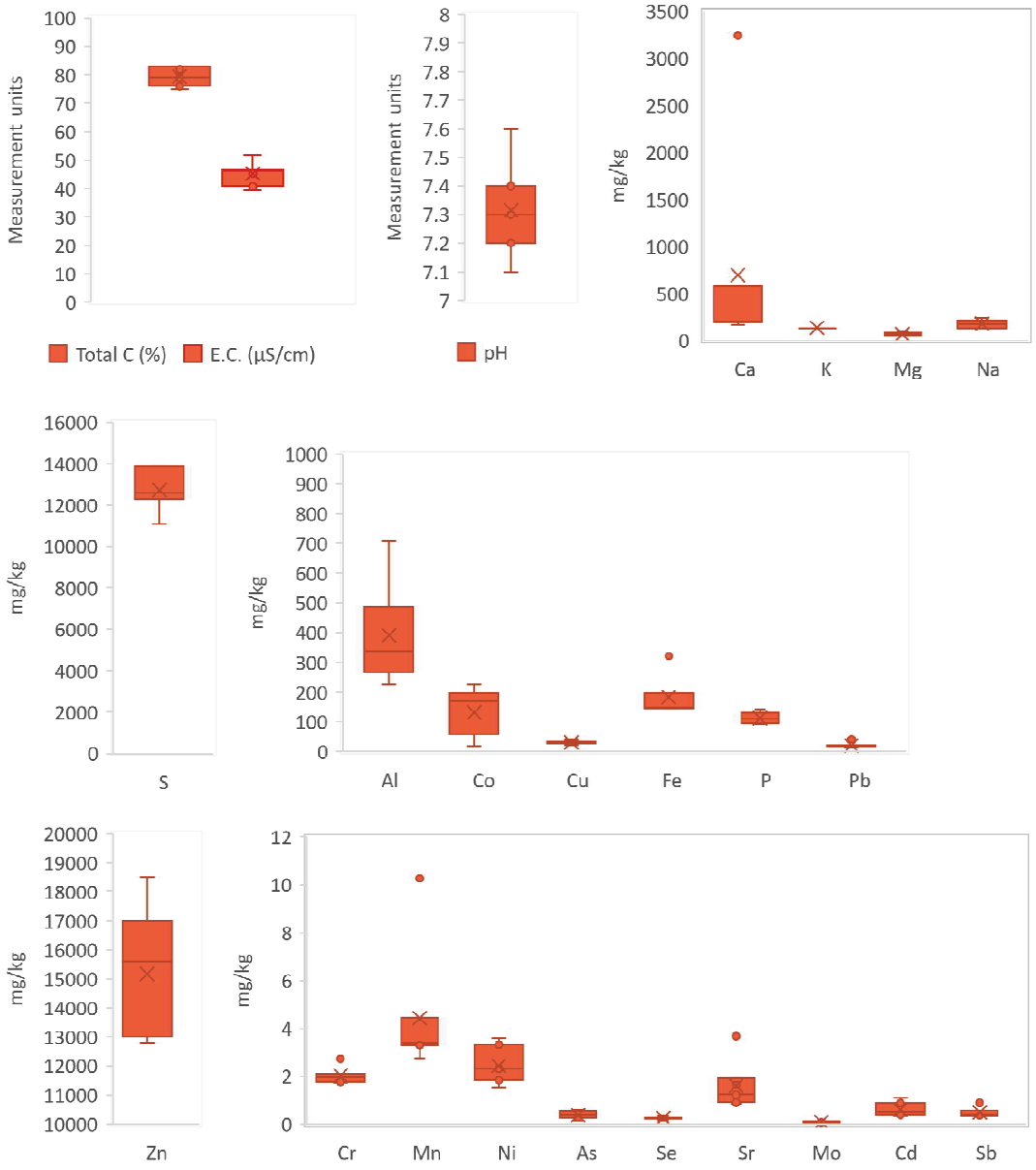

Figure 4 Summary of the elemental analysis for subsamples of recycled rubber product (n=7) shown as box plots to demonstrate sample homogeneity and the potential impact of sample variability on the quality of data generated in this study. Outliers were not removed. Other elements measured but not detected include K (<125 mg/kg for n=6, 132 for n=1), B (<12.5 mg/kg for n=7), and Na (<125 mg/kg for n=2). Average ± standard deviations are in Table 6.

Table 8 Assessment of 6PPD-Q analysis in size reduced samples of recycled rubber product

Sub-sample ID (Size Fraction)	6PPD-Q*, µg/kg	CV (%)	Blank, µg/kg
RRS1TP0922 (Coarse, analysed as received, estimated 5 mm)	12049	3.6	<5
RRS1TP0922 (Ground, < 1 µm)	10787	3.2	<5

*Average of n=3 extractions

The difference in concentrations of 6PPD-Q obtained from the extraction of coarse and ground samples were statistically significant (p <0.05), which indicated that particle size has an impact on the extraction of analytes from the recycled rubber product and may influence analytical results. However, the relative percent difference (RPD) between these two measurements (12 %) is within the acceptable limits for duplicate analysis (Table 5, <30 %). The preliminary data generated in this study suggested that particle size may not make an appreciable difference to the measured concentrations of 6PPD-Q, but this would need to be validated for more samples, and for other chemicals to determine if this trend is consistent. As such, the impact of particle size and size reduction in pre-processing of samples from other recycled rubber products or EOL tyres should not be excluded from consideration in analytical plans.

Extraction of the coarse recycled rubber product resulted in the generation of relatively clean extracts when compared with ground samples. Extractions from ground samples required additional clean-up steps (e.g., filtration or SPE) to minimise contamination and effect on the performance of analytical equipment. The preliminary data generated in this study showed that the analytical results did not notably change between the two size fractions assessed, but this would need to be validated for more samples, and for other chemicals to determine if this trend is consistent. However, when planning analytical regimes where no significant difference in results is expected, the larger size fraction products should be analysed first to minimise impacts on instrument performance and data generated.

3.2.4.4 Interlaboratory comparison and validation of results

Comparison of 6PPD-Q analysis was conducted for measurements performed by an external commercial laboratory and CSIRO. The results are shown in Table 9.

Table 9 Interlaboratory comparison of 6PPD-Q in recycled rubber product sample. The RPD (%) calculated for CS-TYRE1 and CS-TYRE2 is relative to data provided by the external laboratory (EF-TYRE).

Laboratory	Method	6PPD-Q, µg/kg	RPD (%)
CSIRO	CS-TYRE1	15,479	19
	CS-TYRE2	12,049	7
Eurofins	EF-TYRE	13,000	

The lowest RPD was achieved using the CS-TYRE2 method, which was based on the same extraction solvent (methylene chloride and acetonitrile) as used by Eurofins. Analysis following the CS-TYRE1 method, where samples were extracted with methanol, and acetone and hexane, resulted in a higher concentration of 6PPD-Q, potentially due to the use of stronger organic solvents. Nevertheless, the RPDs for the data generated using both methods were within the acceptable limits for duplicate analysis (Table 5), particularly when considering the variability of some of the elements from the assessment of variability (Section 2.3.2). The results of the interlaboratory comparison of 6PPD-Q indicate that the methods developed for 6PPD-Q are consistent with a commercial laboratory.

3.2.5 Key findings and challenges

The key findings for the preliminary characterisation of a commercially available recycled rubber product and two e-waste samples include:

– The recycled rubber product and e-waste samples were characterised for a wide range of chemicals. There were up to 253 discrete chemicals and 26 mixtures (e.g., total C, total BDEs, pH, EC) measured. Other chemicals of interest need to be identified, in consultation with the Department to plan for future sample analyses. In addition, this gap in the understanding of chemicals of concern in wastes more broadly could be investigated using less targeted analytical regimes.

– Results from this work generally agreed with what is known in the literature related to chemicals in EOL tyre and rubber materials and e-wastes. However, the number of samples for each waste type was limited. More samples of similar material types are needed to provide a better indication of chemical characteristic trends for EOL tyres and e-waste materials destined for reuse.

– The TRH analysis of both waste samples indicated that the total amount of organic chemicals present in the samples was not fully quantified or characterised using the targeted LC-MS/MS analysis. The use of other analytical methodology for non-targeted analysis, such as high resolution, accurate mass spectrometry (HRAMS) would be required to address this gap.

– The analytical regimes undertaken in RP2 represented a broad suite of organic, inorganic analytes and physicochemical parameters that were relevant for the samples analysed. Some methods incorporated many analytes but with a lower sensitivity such as the NMI 1120 Screen, which analysed for 78 organic compounds with 1-2 mg/kg LORs. Other targeted methods were more sensitive (with lower LORs) but reported fewer analytes. Using this range of analytical suites offers a means of capturing many common or known contaminants in the waste materials. More resource and time-intensive techniques (e.g., HRAMS) can be developed for individual waste types to capture a broader suite of chemicals expected to be present.

– When assessing inorganic (metals) analytical results, sample heterogeneity did not appear to be an issue with either the recycled rubber product or e-waste samples (as received). However, this may not be the case for samples obtained directly from recycling facilities. Measures to ensure samples representative of bulk waste materials are characterised need to be better considered for future samples, especially related to sample collection at waste facilities.

– Validation of data with an external laboratory demonstrated that the 6PPD-Q analysis at CSIRO was acceptable. Further investigation may be needed to improve recovery and validate the method for 6PPD-Q using samples that will be collected from waste facilities.

3.2.6 Implications for complex waste characterisation

The preliminary characterisation of recycled rubber product and e-waste materials generated in RP2 has several implications for the characterisation of other complex waste materials and ongoing research being completed in IP3, including:

– Characterisation of chemicals in waste would require analysis of different groups of compounds, which would mean multiple analysis via different analytical methods. Having screening methods that can capture a range of chemicals would be ideal.

– The current target suite does not appear to cover all the potential chemicals in waste. Whether or not the analysis conducted captures the key chemicals of potential concern is unclear. Further assessment of the suitability of characterisation methods is required.

– The choice of extraction method will likely influence the number and concentration of analytes extracted, detected, and quantified in complex waste materials. The presence of particles from pulverised or otherwise size reduced fractions of waste can impact the total extraction of chemicals, and consideration of available extraction and clean up methods should be undertaken prior to commencing characterisation of waste samples.
– To ensure accuracy and reliability of results, it is recommended to analyse multiple subsamples, if feasible and within budget constraints. It is also recommended to validate analytical results through external laboratories, as a best practice.

4. Analytical method development

4.1 High-Performance Liquid Chromatography-High-Resolution Accurate-Mass Mass Spectrometry (UHPLC MS MS) Method for Analysis of 6PPD-Q, DPG and HMMM in tyre crumb extracts at CSIRO

A method for the analysis of 6PPD-Q, DPG and HMMM by HPLC-MS MS was developed and validated (Method code: CS-TYRE).

4.1.1 Materials

All standards including 6PPD-Q, DPG, HMMM, deuterated surrogate standard (6PPD-Q D5) and atrazine were purchased from HPC Standards GmbH. Stock solutions of 6PPD-Q was prepared by dissolving 10 mg of commercial standard (98.8% purity solid) in 10 mL acetone to achieve a concentration of 1000 mg/L. DPG was prepared by dissolving 25.7 mg of commercial standard in 25 mL acetone to achieve a concentration of 1.028 mg/mL, whilst HMMM was prepared by dissolving 100 mg of commercial standard (94.56% purity solid) in 10 mL of methanol to achieve a concentration of 1000 mg/L. 6PPD-Q D5 was received as a 100 µg/mL solution in acetonitrile and used as is. A 10 mg/L native standard solution consisting of 6PPD-Q, DPG and HMMM was prepared in methanol. a stable isotope solution of 2 mg/L containing 6PPD Q-d5 and Atrazine was prepared in methanol. 500µL of this solution was added to the tire crumb samples, including the blank samples.

For analysis, eluents used were 0.1 % (v/v) formic acid 10 mM Ammonium Formate and HPLC grade methanol (99.99 %). Chemicals were purchased from Fisher Scientific and ultrapure water was obtained with Q-POD® Ultrapure Water Remote Dispenser with Millipak® 0.22 µm filter.

4.1.2 Extraction

In this experiment, 100 mg samples of recycled rubber product were weighed and placed into a clean and dry amber 10 mL glass tubes. Each sample (coarse and ground) was prepared as 4 replicates. As part of spike recovery testing, another 3 replicates were prepared for the coarse and ground tyre crumb but spiked with 500 µL of 10 mg/L native standard solution. As part of QA/QC, 2 blank samples (no sample, container only), 2 matrix blanks (sand) were also prepared. All samples were then spiked with 500 µL of 2 mg/L stable isotope mixture. The solvent was evaporated off using a nitrogen blown down unit. To extract the samples, a 2.5 mL aliquot of acetonitrile was added to the samples, vortex mixed then placed on a bath sonicator. After 15 minutes, the samples were recovered then centrifuged for 5 minutes at 2000 rpm. The supernatant was transferred into a separate 10-mL container using glass Pasteur pipettes. A second round of extractions were conducted using 2.5 mL of dichloromethane (DCM) following the same ultrasonication and centrifugation procedure. The acetonitrile and the DCM extracts were combined then dried using a gentle stream of nitrogen. The dried extracts were then reconstituted to 1 mL using methanol. As the concentration of these tyre chemicals are expected to be high in the tire crumb samples, the samples were then diluted 50 times with methanol. Extracts were stored at -20 °C until time of analysis.

4.1.3 Analysis

All extracts were analysed by LC-MS/MS. The liquid chromatography system comprised of a Thermo Scientific UltiMate 3000 high-performance liquid chromatography (HPLC) system coupled with TSQ Altis™ Triple Quadrupole Mass Spectrometer, equipped with an ESI probe to be used in the negative and positive ionisation mode. A pre column was also installed after the LC pump and prior to the injection valve to offset background

contaminants from the LC pump, autosampler, degasser, and mobile phases. A guard column has been used prior to the analytical column to any particulates, unwanted compounds, or impurities that may be present in the sample, mobile phase, or any other components of the LC system and improve the performance and accuracy of the liquid chromatography system. The analytical column used for the method was a Hypersil GOLD™ PFP HPLC Column (100 × 2.1 mm, 3 µm particle size) fitted with a preheater for maintaining column temperature (35 °C). The mass spectrometer was operated in positive ion mode, and the transitions used for quantification were m/z 243.0 → 187.0 for 6PPD-Q, m/z 119.1 → 77.1 for DPG, and m/z 359.0 → 177.0 for HMMM (See Table 10).

4.1.4 Quantification

Quantification was conducted using internal standard calibration. The concentration of the standards ranged from 1 to 100 µg/L. Calibration standards were prepared in 100 % methanol, as per samples. So far, the method developed was only able to reliably quantify 6PPD-Q. This method had a LOR of 5 µg/kg (estimated from the LOQ, which is based on 10 times the ratio of the standard deviation of the response and slope of the calibration curve). Recovery of 6PPD-Q based on spike recovery tests following the extraction procedure described was 57 % (Coefficient of Variation =10.5%; n=6). Given that this value is low and close the minimum acceptance criteria (50-150 %; Table 5), results were verified by an external laboratory. Further work is required to optimise and validate this method.

QA/QC samples for HMMM and DPG are problematic hence, are not included in the results. Further investigation is required to improve recovery and validate the method for 6PPD-Q on other samples as well as to confidently quantify problematic compounds at CSIRO.

Table 10 SRM table for the targeted tyre chemical analysis

Compound	Retention Time (RT, min)	Precursor (m/z)	Product (m/z)	Collision Energy (V)
Atrazine*	8.62	216.1	104	28
Atrazine*	8.62	216.1	132	23
HMMM	9.18	391	177	28
HMMM	9.18	391	359	10
1,3 DPG	8.06	212.1	77.1	41
1,3 DPG	8.06	212.1	94	22
6PPD-Q	10.1	299.1	187.1	32
6PPD-Q	10.1	299.1	215	19
6PPD-Q-d5	10.1	304	192	31
66PPD-Q-d5	10.1	304	220.1	19

*Atrazine was chosen as a surrogate standard for HMMM because of its structural similarities.

4.2 Ultra-High-Performance Liquid Chromatography-High-Resolution Accurate-Mass Mass Spectrometry (UHPLC-HRAM MS) Method for Analysis of 38 PFAS at Curtin University

A method for the analysis of 38 PFAS by UHPLC-HRAM MS has been developed and is in the process of being validated for quantification.

4.2.1 Materials

PFAS analytical standards (n=36) and deuterated PFAS analytical standards (n=24) were purchased from Wellington Laboratories, Canada. Trifluoroacetic acid and perfluoropropionic acid were purchased from Sigma Aldrich, Australia. Stock solutions of the individual 38 PFAS were prepared in methanol (50-2500 µg/L). Calibration solutions, with concentrations 0.05-10 µg/L, were prepared using serial dilutions of the stock solution in 50:50 (v/v) methanol/water containing 0.1 % acetic acid.

4.2.2 Extraction

Samples were extracted twice with methanol (100 mg sample to 2.5 mL methanol, total solution 5 mL), followed by two sequential extractions with 1:1 hexane:acetone (2.5 mL each). Supernatants were dried under nitrogen, reconstituted with methanol, and the dark-coloured extract was applied to a solid-phase extraction (SPE) cartridge (Supelco ENVI-18, 500 mg, 3 mL tube, preconditioned with methanol). Eluents were combined and dried under nitrogen. To minimise PFAS contamination, HDPE vials and bottles, rather than glass, were used; vials, tubes, pipette tips were disposed of after use, rather than cleaned and re-used; and the workbench was cleaned with methanol before sampling and extraction.

4.2.3 Analysis

The liquid chromatography system was comprised of a Thermo Scientific™ Vanquish™ flex ultra-high-performance liquid chromatography (UHPLC) system fitted with a Thermo Scientific™ PFC-free kit, and was interfaced with an Orbitrap Exploris 120, HRAMS, equipped with an ESI probe used in the negative or positive ionisation modes for PFAS analysis. An isolator column was also installed after the LC pump and prior to the injection valve to offset background contaminants from the LC pump, autosampler, degasser, and mobile phases. The analytical column used was a Waters C18 2.1 × 100 mm column with a 2.5 µm particle size and was fitted with a preheater for maintaining column temperature (45 °C). All eluents were LC grade solvents. PFAS were detected using UHPLC-HRAM MS. Full method blanks and solvent blanks were included with each analysis.

4.2.4 Future Development

Future research will involve validating this analytical method for the quantitative analysis of PFAS in tyres and e-waste, including incorporation of deuterated surrogate standards. The possibility of including a bistriflimide analyte is being explored. The PFAS extraction method described in US EPA Method 1633 3rd Revision [26] will be developed at Curtin, since this is the extraction method used by Eurofins, thus allowing interlaboratory comparisons to be conducted. Curtin also has the potential to do total organic fluorine analysis in future.

4.3 Ultra-High-Performance Liquid Chromatography-High-Resolution Accurate-Mass Mass Spectrometry (UHPLC-HRAM MS) Method for Analysis of 11 Benzotriazoles and Benzothiazoles at Curtin University

Following on from existing methods for the analysis of a small set of benzotriazoles and benzothiazoles at Curtin University, a method for the analysis of 11 benzotriazoles and benzothiazoles by UHPLC-HRAMS is being developed and validated. Four new benzothiazoles (2-mercaptobenzothiazole, 2-methylthiobenzothiazole, benzothiazole-2-sulfonic acid and 2,2'-dithiobisbenzothiazole) have been chosen because they have previously been reported as components of tyres [24].

4.3.1 Materials

The 11 benzotriazoles and benzothiazoles were all purchased from Sigma Aldrich. The deuterated surrogate standard 5-methylbenzotriazole-D6 was purchased from Toronto Research Chemicals. Eluents used were formic acid (99 %), which was purchased from Thermo Fisher, ultrapure water and methanol (99.99 %), which were both purchased from Honeywell.

4.3.2 Extraction

As described in previous subsection 4.2.

4.3.3 Analysis

The liquid chromatography system was comprised of a Thermo Scientific™ Vanquish™ flex ultra-high-performance liquid chromatography (UHPLC) system interfaced with an Orbitrap Exploris 120 HRAMS, equipped with an H-ESI probe to be used in the negative and positive ionisation mode. An isolator column was also installed after the LC pump and prior to the injection valve to offset background contaminants from the LC pump, autosampler, degasser, and mobile phases. The analytical column used for the method was a Phenomenex Kinetex C18 column (100 × 2.1 mm, 2.6 µm particle size, 100 Å pore size) fitted with a preheater for maintaining column temperature (45 °C).Method development involved optimisation of eluents, ESI polarity and collision energy, as well as choice of precursor and product ions for each analyte (**Error! Reference source not found.**).

4.3.4 Preliminary Results

Preliminary (qualitative only) analysis of the extracts from the recycled rubber product identified the presence of benzothiazole, 2-aminobenzothiazole, 2-methylbenzothiazole, 2-amino-6-hydroxybenzothiazole, 2-methylthiobenzothiazole, 2-mercaptobenzothiazole and benzothiazole-2-sulfonic acid.

4.3.5 Future Development

Further analysis will be conducted on the recycled rubber product sample where an increased extraction of analytes should be achieved. Further method development will be conducted to enable quantification of analytes, as well as determination of LORs and analyte recovery efficiency using an increased number of surrogate standards and spikes.

5. Preliminary leaching methodology for RP3 and beyond

The leachability and release of chemicals from waste materials such as e-waste, EOL tyres and secondary materials sourced from waste-derived materials are not well defined. Standard leaching methodologies are designed for ecological niches or landfills and are not designed for complex waste materials. Hence, the application of standard leaching methodology for these materials has not been established and validated.

A draft leaching methodology has been developed for implementation in RP3 and beyond to assess the availability of chemicals from EOL tyres and e-waste materials using both:

1. Standard leaching methodology such as the Australian Standard Leaching Protocol (ASLP) to the leaching of these materials; and
2. Non-standard leaching methodology that may be more suited to the materials and to application domains of national and/or jurisdictional interests.

The data generated by standard and non-standard leaching assessments provide two things: (i) chemical species that are leachable from the waste that need to be considered for their intrinsic hazard and risk profile, and (ii) leaching fractions from the wastes that may be used in ecotoxicological assessments.
These initial leaching experiments will underpin ongoing assessments of the suitability of leaching methodologies for complex waste materials, with the view of creating a transferrable (but non-prescriptive) guidance document on how to plan and undertake appropriate characterisation assessments of wastes and secondary materials.

The preliminary workflow established for leaching assessments is shown in Figure 5 and summarised in Table 11.

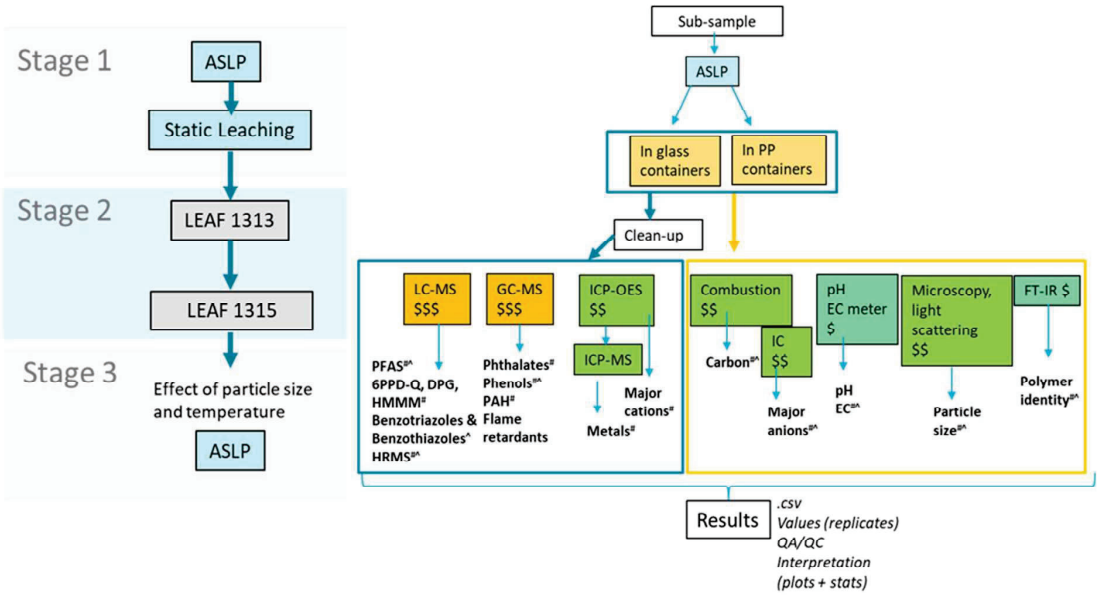

Figure 5 Preliminary workflow for leaching assessment of EOL tyres and e-waste and analytical methods and targets.

Table 11 Summary of preliminary leaching conditions that may be assessed during RP3

Method Number	Method Name	L/S ratio	Tumbling time (hrs)	Equilibration time	pH initial solution	Temperature (°C)	Comments	Modifications	References
1	ASLP - Saturate, tumble and spin	20:1	18	18 h	3, 5, 7 or 9 (dictated by landfill pH, or pH in reuse or recycle pathways of waste materials)	22 ± 5 °C	Standard: no pre-titrations involved; typically assessed at 1 pH condition. Estimates maximum potential release under aggressive leaching conditions. Simulates leaching from improperly designed landfill.	May consider higher pH for initial solutions for e-waste and recycled rubber material. Smaller sample mass may need to be used (from 100 g to 2 g), ensuring the L/S ratio is maintained.	[43]
2	LEAF 1313 - Saturate, tumble and spin	10:1	24	24, 48 or 72 h, depending on max particle size	2 to 12	20 ± 2 °C	Standard: pH of the material is adjusted using pre-titration data; typically assessed at 5 pH conditions.	May consider a smaller range of pH values (e.g., 3-10) that are relevant environmentally, or from application/recycling point of view. Smaller sample mass may need to be used (from 100g to 2g), ensuring the L/S ratio is maintained.	[44]
3	Static leaching / Saturate, stand and spin	3:1	0	4, 8, 24 h	7	20 ± 2 °C	Non-standard: a static batch test under minimal liquid/soil ratio (non-standard) to assess leaching from materials with smaller particle sizes. Simulated conditions most closely reflects environmental conditions.		[45]
4	LEAF 1315 – monolith	L/A ratio 9 mL/cm^2.	0	Sequential intervals of 2 h, 23 h, 5 d, 7 d, and 14 d	7	20 ± 2 °C	Undertake if seeking to scale up towards whole tyres or larger e-waste fragments.		[46, 47]

6. Data management

6.1 Data management strategy for IP3

The data generated from IP3 will be designed to meet the principles outlined in the FAIR Guiding Principles for scientific data management stewardship [48] and National Principles for Environmental Management [49]. Noting that there will be a high volume of analytical data generated throughout the life of this project, a preliminary Data Management Strategy outlining the requirements for the management, reporting and communication of data generated throughout the life of IP3 (and into perpetuity) was initiated at the start of RP2. The document was not designed to be a static document but was intended to be modified and curated as the IP3 research team generates data and deliverables throughout the life of the Hub.

We have prescribed preliminary metadata standards (including codified sample identification, chain of custody methods and documents, and sample metadata), QA/QC standard instructions for our analytical laboratories to ensure data quality and interlaboratory comparisons, and how to report data to the Department using appropriate identifiers linked to chemical synonyms (e.g., CAS RN).

At the time of the development of our strategy, the SCaW Hub did not have a Data Wrangler to assist with the development of our data management tools and strategies. In February 2023, we engaged with Anirban Ghose (University of New South Wales) to assist with the management of data generated, and to ensure that data management strategies were consistently applied across the SCaW Hub. We will continue to co-design our data management strategy and reporting tools as the project progresses.

6.2 Co-designed iterative data reporting template

An iterative data reporting template was provided by the Department and refined with the CSIRO and Curtin University analytical teams. The use of the data reporting template will ensure data generated in RP2 and beyond can be readily used and integrated with other chemical management platforms, and that data sources and quality are traceable with the association of metadata, sample information and analytical information. The use of this data reporting template will also ensure that the data generated throughout IP3 is in an interoperable format suitable for incorporation into a variety of data analytic software.

Information that was initially collected in the data reporting template is summarised in Table 12, and broadly included sample metadata (including photographs and notes related to physical descriptions), a list of chemicals analysed, a description of methods used, analytical data, along with a description of QA/QC information available for each analytical batch. Raw data received from different laboratories were compiled and catalogued to enable future access.

Through further co-design and as more analytical data is generated in IP3, the data reporting template will be iteratively updated to streamline data entry and minimise the risk of data handling errors. Some key recommendations for improvements to the first version of the data management template include:

– Adapting the template to be more intuitive to the user;

– Identify and define critical metadata to include in reporting; and,

– Investigate how to better collect information and data on chemical mixtures.

In addition, some further development of instructional guidelines for using the data reporting template and the development of minimum reporting standards for external laboratories will be investigated throughout RP3.

Table 12 Summary of metadata collected for the data management tool developed by the Department and CSIRO and Curtin University analytical researchers

Chemical	Sample	Method	Batch	Results
CAS RN	Sample ID	Method ID	Batch ID	Batch ID
CAS RN unhyphenated	Sample Description	Description	Method ID	Method ID
Systematic name	Date Sampled	Technique	Date Analysed	Sample ID
Synonym	Waste Stream	Analyte Group	Laboratory	Sample Description
Acronym	Product	Notes	QAQC Description	CASRN
Chemical Type	Age		Notes	Synonym
Limit Value	Component			Prefix
Limit Term	Replicate			Result
Unit	Resin Type			Limit Value
Notes	Origin			Limit Term
SMILES Codes	Sampling Campaign Notes			Unit
				Laboratory Notes

Potential data sensitivities will be discussed with the SCaW Data Wrangler and research users at the Department.

6.3 Emerging research priority – data reporting standards

Information from commercial laboratories with respect to methods used for sample characterisation are not typically available unless requested. Furthermore, analytical results and QA/QC information are typically provided as PDF documents, requiring time-consuming manual entry of information into the data reporting template. Through engagement with the SCaW Hub Data Wrangler, we note that this challenge is one that several IP areas are struggling with, especially researchers undertaking plastic and microplastic related research in IP2.

To ensure data that is received from external sources is accessible and that QA/QC information can be validated, the analytical team will propose a minimum standard for reporting that can be included in requests for services from analytical laboratories. A minimum standard for reporting may include:

– Provision of raw data in accessible format (.csv or .xlsx) alongside .pdf reports;
– Provision of information related to methodology and methodology modifications that may impact data integrity; and,
– Provision of QA/QC methodology.

A minimum standard for reporting data from external laboratories could be adopted as a SCaW Hub-wide initiative to ensure consistency in the data received, and that the data generated throughout the Hub meets FAIR principles.

6.4 Emerging research priority - non-target analysis for waste characterisation

The analytical work planned and completed for IP3 to date has focussed on characterisation and method development for targeted chemicals that are known or suspected to cause harm to environmental and human health. We note that there are likely to be a large suite of chemicals that will remain non-detected through the initial stages of our characterisation studies and will investigate the application of non-target analysis to enable their identification and assessment for chemical prioritisation.

7. Collaboration and capacity building

7.1 External

Through collaborative engagement in 2022, the IP3 research team have been able to secure additional funding ($50 K) from the Victorian Department of Energy, Environment and Climate Action (DEECA) to enhance the scope of research undertaken in 2023. The funding from DEECA is likely to:

- Enhance the suite of chemicals for analysis related to the characterisation of e-wastes;
- Identify gaps in knowledge about the volatility of chemicals associated with e-wastes; and,
- Consider how these chemicals might behave under a defined set of experimental conditions that are relevant to DEECA.

The findings of this scope of work will be presented in a short report to DEECA and will be included in future IP3 annual reports.

In RP2, we engaged with Tyre Stewardship Australia (TSA) to understand how the research priorities for IP3 related to the research direction of TSA. The TSA connected the IP3 analytical team with other researchers at RMIT University and consultants who are also conducting research into the chemical characterisation of tyres and EOL tyres. This engagement will facilitate the sharing of knowledge and challenges related to analytical methodology and the alignment of research priorities for this waste stream. This formal engagement is likely to occur across the life of the Hub to ensure that the research from IP3 is communicated to relevant industry partners and capacity related to the characterisation of tyres and their wastes can be consolidated.

As part of our commitment to ensuring the accuracy and reliability of our results, we have engaged two external laboratories to conduct some of the required analyses for our project and to validate analyses completed internally. Our experience with the data received so far has been positive, and we are now taking steps to further streamline our data reporting process. Specifically, we plan to submit a formal request for data reporting requirements including details on analytical methodology, that will enable us to efficiently enter the information we receive from external laboratories into our data reporting template.

7.2 Cross-Hub engagement

Research activities related to tyres and EOL tyres are currently being undertaken across IP2, IP3 and IP5 within the SCaW Hub. To better consolidate the SCaW Hub research impact in the management of EOL tyres, an initial cross-IP workshop was held between the leaders of IP2, IP3 and IP5 to ensure that research priorities aligned and that there was no duplication of effort.

It is clear from initial engagement that there should be a SCaW Hub-wide research position on EOL tyres management, and there is an opportunity to broadly communicate the outcomes and deliverables of each of the IP2, IP3 and IP5 research activities in a consolidated manner to raise the reputation of the Hub and the research in this space.

7.3 Participating research organisations

The research activities in IP3 will be used to inform the teaching within two new units titled “Chemistry for Sustainability” (CHEM2008; commencing 2023) and “Sustainable Chemistry in Industry” (CHEM3000; commencing 2024) within the new Chemistry of Sustainability Specialisation in the BSc Chemistry Major at Curtin University. CHEM2008 will be available to a wide group of students, since it is available to students who have studied ATAR Chemistry at a minimum.

A/Prof Robert Niven has incorporated elements of the IP3 program and other independent studies of tyre wastes into the course ZEIT4604 Hydrology and Environmental Engineering Practice, taught to fourth-year BE (Civil) (Hons) students at UNSW Canberra.

Dr Mitzi Bolton secured a Masters by Coursework student focussing on the application of Artificial Intelligence in Hazardous Waste Management. Though not funded directly by the NESP SCaW Hub, this was identified as a key tool for improving screening and detection of emerging hazardous wastes priorities using machine learning and will contribute broadly to sharing of information related to waste characterisation and prioritisation objectives of IP3.

Dr Naomi Boxall has been invited to give a guest lecture related to Managing Problematic Wastes as part of the Masters of Environment and Climate Emergency at Curtin University.

8. Risk management

8.1 Health, safety and environment

The research proposed in IP3 is targeting waste samples with largely unknown chemical composition. As a result, both analytical laboratories have conducted risk assessments and have controls in place to protect the health and safety of personnel and to ensure that there is no accidental release to the environment or damage to analytical equipment. Risk assessments considered the following, with the view of developing general HSE documents that covered multiple waste types:

– General laboratory risks;

– Risks associated with materials of unknown composition;

– Risks associated with materials in fine powder (e.g., from pulverised e-waste materials);

– Risks associated with sample preparation and extraction; and,

– Risks associated with use of instrumentation and equipment.

In addition, HSE considerations have also been built into the sampling guidance document to ensure that sampling of waste products with unknown chemical composition is undertaken in a safe manner.

8.2 Sample procurement

As part of RP2, it was proposed that the analytical team would be able to acquire samples of recycled material to characterise from industry partners. This aspect of industry engagement has proven challenging, and to date, we have been unable to secure samples through direct industry engagement and collaboration. As a result, the characterisation data presented for RP2 pertains to the analysis of a commercially available recycled rubber product, and samples of e-waste that were sourced from CSIRO's sample repository. Access to samples were limited for this preliminary screening and comparison with literature values were used to demonstrate results were within expected ranges.

The repository and commercially purchased samples have been instrumental in developing baseline data related to the chemical composition of these wastes and have been crucial in the development of analytical methods, interlaboratory validation of methods and data, the development of preliminary sampling guidance materials and data management tools, and the methodology for leaching to be implemented in later research. Through continued liaison with industry representatives (i.e., stewardship bodies), we will endeavour to obtain suitable recycled and second use materials for characterisation that will not compromise the generation of high quality analytical data.

8.3 Engagement and due diligence

Managing the real or perceived risks for industry participation in IP3 has been a challenge that has directly impacted securing collaboration and samples for analysis in RP2. There are implications for industry in understanding the chemical composition and potential risks associated with secondary materials for establishing or existing markets, and these need to be understood and managed moving forward. Information about the detection, quantification, and associated risk of some chemicals in waste products that are already in use can trigger alarm and scrutiny, and data generated in this project has the potential to influence decisions that may disrupt or promote established market pathways, particularly related to recycled rubber materials.

In addition, it was flagged by the Department that the IP3 project team need to undertake appropriate due diligence when establishing collaborative partnerships with industry to ensure that reputations of the research team (and their associated organisations), the SCaW Hub and the Department would not be incidentally compromised because of this engagement. We can confirm that there are no issues or concerns related to the status of current collaborative partners. However, where required, the project team will de-identify information relating to industry partners in public facing documents. All collaborative partnerships established will now go through a basic due diligence process that will be carried out internally by business development officers at CSIRO.

8.4 Indigenous Engagement

The effect of hazardous wastes on the health, cultural, social, and economic well-being of Indigenous communities needs to be quantified and offers a significant research opportunity. RP2 includes an emphasis on characterising the human and environmental risks of wastes that may be in and near to remote and rural communities, including Indigenous communities. Tyres and electronic goods are commonly used in regions, potentially leaving waste legacies. It is anticipated that better understanding of the total, leachable, and bioavailable chemical components of tyres and e-waste, will support enhanced management and reuse of these waste streams, and identification of potential employment and market opportunities for Indigenous communities.

Given the laboratory-based nature, early status and regulatory drive of the work proposed in RP2, the project was considered a Category 3 Project under the NESP2 SCaW Hub Indigenous Partnerships Strategy, where data and outcomes generated will be communicated and shared to relevant Indigenous organisations, as necessary, and this has not yet been identified.

We recognise still that all work undertaken, irrespective of its nature, will have beneficial outcomes for Indigenous Australians, as we communicate and share findings with relevant groups, and identify research priorities related to IP3 that have both interest and value to Indigenous communities. This involves structuring future research plans to better co-design, collaborate and communicate the outcomes in partnership with Indigenous people, organisations, and communities, with the ultimate goal of strengthening dialogue and participation, increasing Indigenous research capabilities, and supporting Indigenous-led research related to Hazardous Waste, Substances and Pollutants.

Participants in this research team have already completed (or will be requested to complete in the case of new members) the training related to Indigenous Cultural and Intellectual Property. All engagement, regardless of the content or intent, will be guided through the SCaW Hub Indigenous Facilitators, and any traditional knowledge and intellectual property will be managed in accordance with the Indigenous Partnerships Strategy.

9 IP3 horizon of work for 2023 and beyond

RP3 (2023-2024) for IP3 will build on the strong research foundation generated by RP1 and RP2 to continue to provide data and methodologies for the characterisation of risks associated with identified chemicals in EOL tyres and e-waste.

RP3 has three focus areas:

1) To validate sampling and analytical strategies by intensifying analysis of targeted e-waste and EOL tyre components focused on quantification of chemical concentrations and mass in wastes.
2) To establish the leachable chemical fractions from the waste streams and/or repurposed materials to inform risk assessments and handling.
3) To establish methodologies for ecotoxicological studies that may be warranted based on leachable chemicals from e-waste and EOL tyre components.

The proposal for RP3 has been approved for commencement, with contracting to be completed soon. The time horizon foreseen to address hazardous waste challenges related to IP3 is shown in Figure 6.

Figure 6 Time horizon for Impact Priority 3 (Hazardous Waste, Substances and Pollutants).

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Appendix 1 – Summary of relevant analyte groups and identifiers

Analytes with CASRN and other systematic identifiers

CASRN	Group	Systematic name	Synonym
121-14-2	Amines Nitroaromatics & Nitrosamines	1-Methyl-2,4-dinitrobenzene	2,4-Dinitrotoluene
606-20-2	Amines Nitroaromatics & Nitrosamines	2-Methyl-1,3-dinitrobenzene	2,6-Dinitrotoluene
88-74-4	Amines Nitroaromatics & Nitrosamines	2-Nitroaniline	2-Nitroaniline
99-09-2	Amines Nitroaromatics & Nitrosamines	3-Nitroaniline	3-Nitroaniline
106-47-8	Amines Nitroaromatics & Nitrosamines	4-Chloroaniline	4-Chloroaniline
100-01-6	Amines Nitroaromatics & Nitrosamines	4-Nitroaniline	4-Nitroaniline
2395-99-5	Amines Nitroaromatics & Nitrosamines	4-Nitrophenyl	Nitrobenzene
62-53-3	Amines Nitroaromatics & Nitrosamines	Aniline	Aniline
103-33-3	Amines Nitroaromatics & Nitrosamines	Diphenyldiazene	Azobenzene
62-75-9	Amines Nitroaromatics & Nitrosamines	N-Methyl-N-nitrosomethanamine	N-Nitrosodimethylamine
89017-33-4	Amines Nitroaromatics & Nitrosamines	N-Nitroso-1-propanamine	N-Nitrosodi-n-propylamine
86-30-6	Amines Nitroaromatics & Nitrosamines	N-Nitroso-N-phenylaniline	N-Nitrosodiphenylamine
1163-19-5	Brominated ~~e~~diphenyle ~~E~~thers	Benzene, 1,1'-oxybis[2,3,4,5,6-pentabromo- (9CI, ACI)	BDE 209
117964-21-3	Bromodiphenyl Ethers	Benzene, 1,1'-oxybis[2,3,4,6-tetrabromo- (9CI, ACI)	BDE 197
68631-49-2	Bromodiphenyl Ethers	Benzene, 1,1'-oxybis[2,4,5-tribromo- (9CI, ACI)	BDE 153
93703-48-1	Bromodiphenyl Ethers	Benzene, 1,1'-oxybis[3,4-dibromo- (9CI, ACI)	BDE 77
63387-28-0	Bromodiphenyl Ethers	Benzene, 1,2,3,4,5-pentabromo-6-(2,3,4,5-tetrabromophenoxy)- (ACI)	BDE 206
437701-79-6	Bromodiphenyl Ethers	Benzene, 1,2,3,4,5-pentabromo-6-(2,3,4,6-tetrabromophenoxy)- (ACI)	BDE 207
437701-78-5	Bromodiphenyl Ethers	Benzene, 1,2,3,4,5-pentabromo-6-(2,3,5,6-tetrabromophenoxy)- (ACI)	BDE 208
337513-72-1	Bromodiphenyl Ethers	Benzene, 1,2,3,4,5-pentabromo-6-(2,4,5-tribromophenoxy)- (ACI)	BDE 203
446255-54-5	Bromodiphenyl Ethers	Benzene, 1,2,3,4,5-pentabromo-6-(2,4,6-tribromophenoxy)- (ACI)	BDE 204
446255-56-7	Bromodiphenyl Ethers	Benzene, 1,2,3,4,5-pentabromo-6-(3,4,5-tribromophenoxy)- (ACI)	BDE 205
446255-39-6	Bromodiphenyl Ethers	Benzene, 1,2,3,4-tetrabromo-5-(2,3,4,6-tetrabromophenoxy)- (9CI, ACI)	BDE 196
446255-26-1	Bromodiphenyl Ethers	Benzene, 1,2,3,4-tetrabromo-5-(2,4,5-tribromophenoxy)- (9CI, ACI)	BDE 180
446255-19-2	Bromodiphenyl Ethers	Benzene, 1,2,3,5-tetrabromo-4-(2,3,4-tribromophenoxy)- (9CI, ACI)	BDE 171
446255-50-1	Bromodiphenyl Ethers	Benzene, 1,2,3,5-tetrabromo-4-(2,3,5,6-tetrabromophenoxy)- (9CI, ACI)	BDE 201

CASRN	Group	Systematic name	Synonym
207122-16-5	Bromodiphenyl Ethers	Benzene, 1,2,3,5-tetrabromo-4-(2,4,5-tribromophenoxy)- (9CI, ACI)	BDE 183
117948-63-7	Bromodiphenyl Ethers	Benzene, 1,2,3,5-tetrabromo-4-(2,4,6-tribromophenoxy)- (9CI, ACI)	BDE 184
446254-96-2	Bromodiphenyl Ethers	Benzene, 1,2,3,5-tetrabromo-4-(2,4-dibromophenoxy)- (9CI, ACI)	BDE 139
446255-30-7	Bromodiphenyl Ethers	Benzene, 1,2,3,5-tetrabromo-4-(3,4,5-tribromophenoxy)- (9CI, ACI)	BDE 191
243982-83-4	Bromodiphenyl Ethers	Benzene, 1,2,3-tribromo-4-(2,4,6-tribromophenoxy)- (9CI, ACI)	BDE 140
182346-21-0	Bromodiphenyl Ethers	Benzene, 1,2,3-tribromo-4-(2,4-dibromophenoxy)- (9CI, ACI)	BDE 85
366791-32-4	Bromodiphenyl Ethers	Benzene, 1,2,3-tribromo-5-(3,4-dibromophenoxy)- (9CI, ACI)	BDE 126
60348-60-9	Bromodiphenyl Ethers	Benzene, 1,2,4-tribromo-5-(2,4-dibromophenoxy)- (9CI, ACI)	BDE 99
189084-61-5	Bromodiphenyl Ethers	Benzene, 1,2-dibromo-4-(2,4-dibromophenoxy)- (9CI, ACI)	BDE 66
207122-15-4	Bromodiphenyl Ethers	Benzene, 1,3,5-tribromo-2-(2,4,5-tribromophenoxy)- (9CI, ACI)	BDE 154
189084-64-8	Bromodiphenyl Ethers	Benzene, 1,3,5-tribromo-2-(2,4-dibromophenoxy)- (9CI, ACI)	BDE 100
189084-66-0	Bromodiphenyl Ethers	Benzene, 1,3,5-tribromo-2-(3,4-dibromophenoxy)- (9CI, ACI)	BDE 119
155999-95-4	Bromodiphenyl Ethers	Benzene, 1,3,5-tribromo-2-phenoxy- (9CI, ACI)	BDE 30
189084-62-6	Bromodiphenyl Ethers	Benzene, 1,3-dibromo-2-(3,4-dibromophenoxy)- (9CI, ACI)	BDE 71
243982-82-3	Bromodiphenyl Ethers	Benzene, 1,4-dibromo-2-(2,4-dibromophenoxy)- (9CI, ACI)	BDE 49
5436-43-1	Bromodiphenyl Ethers	Benzene, 2,4-dibromo-1-(2,4-dibromophenoxy)- (ACI)	BDE 47
147217-75-2	Bromodiphenyl Ethers	Benzene, 2,4-dibromo-1-(2-bromophenoxy)- (9CI, ACI)	BDE 17
7440-44-0	Carbon	Carbon	Total C
101-55-3	Ethers	1-Bromo-4-phenoxybenzene	4-Bromophenyl phenyl ether
111-44-4	Ethers	1-Chloro-2-(2-chloroethoxy)ethane	Bis(2-chloroethyl)ether
111-91-1	Ethers	1-Chloro-2-[(2-chloroethoxy)methoxy]ethane	Bis(2-chloroethoxy)methane
7005-72-3	Ethers	1-Chloro-4-phenoxybenzene	4-Chlorophenyl phenyl ether
39638-32-9	Ethers	2-Chloro-2-[(2-chloro-2-propanyl)oxy]propane	Bis(2-chloroisopropyl)ether
10061-02-6	Halogenated Aliphatic Hydrocarbons	(1E)-1,3-Dichloro-1-propene	trans-1,3-Dichloropropene
10061-01-5	Halogenated Aliphatic Hydrocarbons	(1Z)-1,3-Dichloro-1-propene	cis-1,3-Dichloropropene
156-60-5	Halogenated Aliphatic Hydrocarbons	(E)-1,2-Dichloroethene	trans-1,2-Dichloroethene
156-59-2	Halogenated Aliphatic Hydrocarbons	(Z)-1,2-Dichloroethene	cis-1,2-Dichloroethene
630-20-6	Halogenated Aliphatic Hydrocarbons	1,1,1,2-Tetrachloroethane	1,1,1,2-Tetrachloroethane
71-55-6	Halogenated Aliphatic Hydrocarbons	1,1,1-Trichloroethane	1,1,1-Trichloroethane

CASRN	Group	Systematic name	Synonym
79-34-5	Halogenated Aliphatic Hydrocarbons	1,1,2,2-Tetrachloroethane	1,1,2,2-Tetrachloroethane
87-68-3	Halogenated Aliphatic Hydrocarbons	1,1,2,3,4,4-Hexachloro-1,3-butadiene	Hexachlorobutadiene
79-00-5	Halogenated Aliphatic Hydrocarbons	1,1,2-Trichloroethane	1,1,2-Trichloroethane
79-01-6	Halogenated Aliphatic Hydrocarbons	1,1,2-Trichloroethene	Trichloroethene
563-58-6	Halogenated Aliphatic Hydrocarbons	1,1-Dichloro-1-propene	1,1-Dichloropropene
75-34-3	Halogenated Aliphatic Hydrocarbons	1,1-Dichloroethane	1,1-Dichloroethane
75-35-4	Halogenated Aliphatic Hydrocarbons	1,1-Dichloroethene	1,1-Dichloroethene
77-47-4	Halogenated Aliphatic Hydrocarbons	1,2,3,4,5,5-Hexachloro-1,3-cyclopentadiene	Hexachlorocyclopentadiene
96-18-4	Halogenated Aliphatic Hydrocarbons	1,2,3-Trichloropropane	1,2,3-Trichloropropane
96-12-8	Halogenated Aliphatic Hydrocarbons	1,2-Dibromo-3-chloropropane	1,2-Dibromo-3-chloropropane
106-93-4	Halogenated Aliphatic Hydrocarbons	1,2-Dibromoethane	1,2-Dibromoethane
107-06-2	Halogenated Aliphatic Hydrocarbons	1,2-dichloroethane	1,2-Dichloroethane
78-87-5	Halogenated Aliphatic Hydrocarbons	1,2-Dichloropropane	1,2-Dichloropropane
142-28-9	Halogenated Aliphatic Hydrocarbons	1,3-Dichloropropane	1,3-Dichloropropane
594-20-7	Halogenated Aliphatic Hydrocarbons	2,2-Dichloropropane	2,2-Dichloropropane
74-97-5	Halogenated Aliphatic Hydrocarbons	Bromochloromethane	Bromochloromethane
74-83-9	Halogenated Aliphatic Hydrocarbons	Bromomethane	Bromomethane
75-00-3	Halogenated Aliphatic Hydrocarbons	Chloroethane	Chloroethane
75-01-4	Halogenated Aliphatic Hydrocarbons	Chloroethene	Vinyl chloride
74-87-3	Halogenated Aliphatic Hydrocarbons	Chloromethane	Chloromethane
74-95-3	Halogenated Aliphatic Hydrocarbons	Dibromomethane	Dibromomethane
75-09-2	Halogenated Aliphatic Hydrocarbons	Dichloromethane	Dichloromethane
67-72-1	Halogenated Aliphatic Hydrocarbons	Hexachloroethane	Hexachloroethane
127-18-4	Halogenated Aliphatic Hydrocarbons	Tetrachloroethene	Tetrachloroethene
56-23-5	Halogenated Aliphatic Hydrocarbons	Tetrachloromethane	Carbon tetrachloride
75-69-4	Halogenated Aliphatic Hydrocarbons	Trichloro(fluoro)methane	Trichlorofluoromethane
634-66-2	Halogenated Aromatic Hydrocarbons	1,2,3,4-Tetrachlorobenzene	1,2,3,4-Tetrachlorobenzene

CASRN	Group	Systematic name	Synonym
87-61-6	Halogenated Aromatic Hydrocarbons	1,2,3-Trichlorobenzene	1,2,3-Trichlorobenzene
120-82-1	Halogenated Aromatic Hydrocarbons	1,2,4-Trichlorobenzene	1,2,4-Trichlorobenzene
95-50-1	Halogenated Aromatic Hydrocarbons	1,2-Dichlorobenzene	1,2-Dichlorobenzene
541-73-1	Halogenated Aromatic Hydrocarbons	1,3-Dichlorobenzene	1,3-Dichlorobenzene
106-46-7	Halogenated Aromatic Hydrocarbons	1,4-Dichlorobenzene	1,4-Dichlorobenzene
95-49-8	Halogenated Aromatic Hydrocarbons	1-Chloro-2-methylbenzene	2-Chlorotoluene
106-43-4	Halogenated Aromatic Hydrocarbons	1-Chloro-4-methylbenzene	4-Chlorotoluene
91-58-7	Halogenated Aromatic Hydrocarbons	2-Chloronaphthalene	2-Chloronaphthalene
108-86-1	Halogenated Aromatic Hydrocarbons	Bromobenzene	Bromobenzene
108-90-7	Halogenated Aromatic Hydrocarbons	Chlorobenzene	Chlorobenzene
118-74-1	Halogenated Aromatic Hydrocarbons	Hexachlorobenzene	Hexachlorobenzene
24959-67-9	Major anions	Bromide	Br^-
16887-00-6	Major anions	Chloride	Cl^-
16984-48-8	Major anions	Fluoride	F^-
14797-55-8	Major anions	Nitrate	NO_3^-
14808-79-8	Major anions	Sulfate	$SO_4^=$
7440-70-2	Major elements	Calcium	Ca
7439-95-4	Major elements	Magnesium	Mg
7440-09-7	Major elements	Potassium	K
7440-23-5	Major elements	Sodium	Na
7704-34-9	Major elements	Sulfur	S
98-82-8	Monocyclic Aromatic Hydrocarbons	(1-Methylethyl)benzene	Isopropylbenzene
95-63-6	Monocyclic Aromatic Hydrocarbons	1,2,4-Trimethylbenzene	1,2,4-Trimethylbenzene
95-47-6	Monocyclic Aromatic Hydrocarbons	1,2-Dimethylbenzene	o-Xylene
108-67-8	Monocyclic Aromatic Hydrocarbons	1,3,5-Trimethylbenzene	1,3,5-Trimethylbenzene
99-87-6	Monocyclic Aromatic Hydrocarbons	1-Isopropyl-4-methylbenzene	4-Isopropyltoluene
103-65-1	Monocyclic Aromatic Hydrocarbons	1-Phenylpropane	n-Propylbenzene
71-43-2	Monocyclic Aromatic Hydrocarbons	Benzene	Benzene
104-51-8	Monocyclic Aromatic Hydrocarbons	Butylbenzene	n-Butylbenzene
100-42-5	Monocyclic Aromatic Hydrocarbons	Ethenylbenzene	Styrene
100-41-4	Monocyclic Aromatic Hydrocarbons	Ethylbenzene	Ethylbenzene

CASRN	Group	Systematic name	Synonym
108-88-3	Monocyclic Aromatic Hydrocarbons	methylbenzene	Toluene
135-98-8	Monocyclic Aromatic Hydrocarbons	sec-Butylbenzene	sec-Butylbenzene
98-06-6	Monocyclic Aromatic Hydrocarbons	tert-Butylbenzene	tert-Butylbenzene
319-85-7	Organochlorine Pesticides	(1r,2r,3r,4r,5r,6r)-1,2,3,4,5,6-Hexachlorocyclohexane	b-BHC
319-84-6	Organochlorine Pesticides	(1R,2R,3R,4R,5S,6S)-1,2,3,4,5,6-Hexachlorocyclohexane	a-BHC
58-89-9	Organochlorine Pesticides	(1R,2S,3r,4R,5S,6r)-1,2,3,4,5,6-Hexachlorocyclohexane	g-BHC (Lindane)
7421-93-4	Organochlorine Pesticides	1,2,4-Methenocyclopenta[cd]pentalene-5-carboxaldehyde, 2,2a,3,3,4,7-hexachlorodecahydro-, (1R,2R,2aR,4S,4aS,5R,6aR,6bR,7S)-rel- (9Cl, ACI)	Endrin Aldehyde
309-00-2	Organochlorine Pesticides	1R,2R,3R,6S,7S,8S)-1,8,9,10,11,11-Hexachlorotetracyclo[6.2.1.13,6.02,7]dodeca-4,9-diene	Aldrin
1024-57-3	Organochlorine Pesticides	2,5-Methano-2H-indeno[1,2-b]oxirene, 2,3,4,5,6,7,7-heptachloro-1a,1b,5,5a,6,6a-hexahydro-, (1aR,1bS,2R,5S,5aR,6S,6aR)-rel- (9Cl, ACI)	Heptachlorepoxide
72-20-8	Organochlorine Pesticides	2,7:3,6-Dimethanonaphth[2,3-b]oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1aR,2R,2aR,3R,6S,6aS,7S,7aS)-rel- (9Cl, ACI)	Endrin
60-57-1	Organochlorine Pesticides	2,7:3,6-Dimethanonaphth[2,3-b]oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1aR,2R,2aS,3S,6R,6aR,7S,7aS)-rel- (9Cl, ACI)	Dieldrin
76-44-8	Organochlorine Pesticides	4,7-Methano-1H-indene, 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro- (9Cl, ACI)	Heptachlor
115-29-7	Organochlorine Pesticides	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide (9Cl, ACI)	Endosulfan sulphate
33213-65-9	Organochlorine Pesticides	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide, (3α,5aα,6β,9β,9aα)- (9Cl, ACI)	Endosulphan II
959-98-8	Organochlorine Pesticides	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide, (3α,5aβ,6α,9α,9aβ)- (9Cl, ACI)	Endosulphan I
50-29-3	Organochlorine Pesticides	Benzene, 1,1′-(2,2,2-trichloroethylidene)bis[4-chloro- (9Cl, ACI)	4,4 '-DDT
72-55-9	Organochlorine Pesticides	Benzene, 1,1′-(2,2-dichloroethenylidene)bis[4-chloro- (ACI)	4,4 '-DDE
72-54-8	Organochlorine Pesticides	Benzene, 1,1′-(2,2-dichloroethylidene)bis[4-chloro- (9Cl, ACI)	4,4 '-DDD
319-86-8	Organochlorine Pesticides	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1α,2α,3α,4β,5α,6β)- (9Cl, ACI)	d-BHC
121-75-5	Organophosphate Pesticides	Butanedioic acid, 2-[(dimethoxyphosphinothioyl)thio]-, 1,4-diethyl ester (ACI)	Malathion
60-51-5	Organophosphate Pesticides	Phosphorodithioic acid, O,O-dimethyl S-[2-(methylamino)-2-oxoethyl] ester (9Cl, ACI)	Dimethoate

CASRN	Group	Systematic name	Synonym
563-12-2	Organophosphate Pesticides	Phosphorodithioic acid, SP,SP'-methylene OP,OP,OP',OP'-tetraethyl ester (ACI)	Ethion
2921-88-2	Organophosphate Pesticides	Phosphorothioic acid, O,O-diethyl O-(3,5,6-trichloro-2-pyridinyl) ester (9CI, ACI)	Chlorpyrifos
333-41-5	Organophosphate Pesticides	Phosphorothioic acid, O,O-diethyl O-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester (9CI, ACI)	Diazinon
122-14-5	Organophosphate Pesticides	Phosphorothioic acid, O,O-dimethyl O-(3-methyl-4-nitrophenyl) ester (9CI, ACI)	Fenitrothion
1331-47-1	Other Organic Compounds	[1,1'-Biphenyl]-4,4'-diamine, dichloro- (9CI, ACI)	Dichlorobenzidine
78-59-1	Other Organic Compounds	2-Cyclohexen-1-one, 3,5,5-trimethyl- (8CI, 9CI, ACI)	Isophorone
86-74-8	Other Organic Compounds	9H-Carbazole (9CI, ACI)	Carbazole
100-51-6	Other Organic Compounds	Benzenemethanol (9CI, ACI)	Benzyl alcohol
132-64-9	Other Organic Compounds	Dibenzofuran	Dibenzofuran
75-15-0	Other Organic Compounds	Methanedithione	Carbon disulfide
91-57-6	Other Organic Compounds	Naphthalene, 2-methyl- (8CI, 9CI, ACI)	2-Methylnaphthalene
78-93-3	Oxygenated Compounds	2-Butanone	2-Butanone (MEK)
591-78-6	Oxygenated Compounds	2-Hexanone	2-Hexanone (MBK)
1634-04-4	Oxygenated Compounds	2-Methoxy-2-methylpropane	Methyl tert-Butyl Ether (MTBE)
108-10-1	Oxygenated Compounds	4-Methyl-2-pentanone	4-Methyl-2-pentanone (MIBK)
67-64-1	Oxygenated Compounds	Acetone	Acetone
108-05-4	Oxygenated Compounds	Vinyl acetate	Vinylacetate
58-90-2	Phenols	2,3,4,6-Tetrachlorophenol	2,3,4,6-Tetrachlorophenol
95-95-4	Phenols	2,4,5-trichlorophenol	2,4,5-Trichlorophenol
88-06-2	Phenols	2,4,6-Trichlorophenol	2,4,6-Trichlorophenol
120-83-2	Phenols	2,4-Dichlorophenol	2,4-Dichlorophenol
105-67-9	Phenols	2,4-Dimethylphenol	2,4-Dimethylphenol
87-65-0	Phenols	2,6-Dichlorophenol	2,6-Dichlorophenol
95-57-8	Phenols	2-Chlorophenol	2-Chlorophenol
88-75-5	Phenols	2-Nitrophenol	2-Nitrophenol
59-50-7	Phenols	4-Chloro-3-methylphenol	4-Chloro-3-methylphenol
95-48-7	Phenols	o-Cresol	2-Methylphenol
87-86-5	Phenols	Pentachlorophenol	Pentachlorophenol
108-95-2	Phenols	Phenol	Phenol
131-11-3	Phthalates	1,2-Benzenedicarboxylic acid, 1,2-dimethyl ester	Dimethyl phthalate
85-68-7	Phthalates	Benzyl butyl phthalate	Butyl benzyl phthalate
117-81-7	Phthalates	Bis(2-ethylhexyl) phthalate	Bis(2-ethylhexyl) phthalate
84-74-2	Phthalates	Dibutyl phthalate	Di-n-butyl phthalate
84-66-2	Phthalates	Diethyl phthalate	Diethyl phthalate

CASRN	Group	Systematic name	Synonym
117-84-0	Phthalates	Dioctyl phthalate	Di-n-octyl phthalate
2051-24-3	Polychlorinated biphenyls	1,1′-Biphenyl, 2,2′,3,3′,4,4′,5,5′,6,6′-decachloro- (9CI, ACI)	PCB # 209
40186-72-9	Polychlorinated biphenyls	1,1′-Biphenyl, 2,2′,3,3′,4,4′,5,5′,6-nonachloro- (9CI, ACI)	PCB # 206
52663-78-2	Polychlorinated biphenyls	1,1′-Biphenyl, 2,2′,3,3′,4,4′,5,6-octachloro- (9CI, ACI)	PCB # 195
35065-30-6	Polychlorinated biphenyls	1,1′-Biphenyl, 2,2′,3,3′,4,4′,5-heptachloro- (9CI, ACI)	PCB # 170
38380-07-3	Polychlorinated biphenyls	1,1′-Biphenyl, 2,2′,3,3′,4,4′-hexachloro- (9CI, ACI)	PCB # 128
35065-29-3	Polychlorinated biphenyls	1,1′-Biphenyl, 2,2′,3,4,4′,5,5′-heptachloro- (9CI, ACI)	PCB # 180
35065-28-2	Polychlorinated biphenyls	1,1′-Biphenyl, 2,2′,3,4,4′,5′-hexachloro- (9CI, ACI)	PCB # 138
52663-68-0	Polychlorinated biphenyls	1,1′-Biphenyl, 2,2′,3,4′,5,5′,6-heptachloro- (9CI, ACI)	PCB # 187
41464-39-5	Polychlorinated biphenyls	1,1′-Biphenyl, 2,2′,3,5′-tetrachloro- (9CI, ACI)	PCB # 44
35065-27-1	Polychlorinated biphenyls	1,1′-Biphenyl, 2,2′,4,4′,5,5′-hexachloro- (9CI, ACI)	PCB # 153
37680-73-2	Polychlorinated biphenyls	1,1′-Biphenyl, 2,2′,4,5,5′-pentachloro- (9CI, ACI)	PCB # 101
35693-99-3	Polychlorinated biphenyls	1,1′-Biphenyl, 2,2′,5,5′-tetrachloro- (9CI, ACI)	PCB # 52
37680-65-2	Polychlorinated biphenyls	1,1′-Biphenyl, 2,2′,5-trichloro- (9CI, ACI)	PCB # 18
32598-14-4	Polychlorinated biphenyls	1,1′-Biphenyl, 2,3,3′,4,4′-pentachloro- (9CI, ACI)	PCB # 105
31508-00-6	Polychlorinated biphenyls	1,1′-Biphenyl, 2,3′,4,4′,5-pentachloro- (9CI, ACI)	PCB # 118
32598-10-0	Polychlorinated biphenyls	1,1′-Biphenyl, 2,3′,4,4′-tetrachloro- (9CI, ACI)	PCB # 66
7012-37-5	Polychlorinated biphenyls	1,1′-Biphenyl, 2,4,4′-trichloro- (9CI, ACI)	PCB # 28
34883-43-7	Polychlorinated biphenyls	1,1′-Biphenyl, 2,4′-dichloro- (9CI, ACI)	PCB # 8
32774-16-6	Polychlorinated biphenyls	1,1′-Biphenyl, 3,3′,4,4′,5,5′-hexachloro- (9CI, ACI)	PCB # 169
57465-28-8	Polychlorinated biphenyls	1,1′-Biphenyl, 3,3′,4,4′,5-pentachloro- (9CI, ACI)	PCB # 126
32598-13-3	Polychlorinated biphenyls	1,1′-Biphenyl, 3,3′,4,4′-tetrachloro- (9CI, ACI)	PCB # 77
86-73-7	Polycyclic Aromatic Hydrocarbons	9H-Fluorene	Fluorene
208-96-8	Polycyclic Aromatic Hydrocarbons	Acenaphthylene	Acenaphthylene
120-12-7	Polycyclic Aromatic Hydrocarbons	Anthracene	Anthracene
50-32-8	Polycyclic Aromatic Hydrocarbons	Benzo(a)pyrene	Benzo(a)pyrene
191-24-2	Polycyclic Aromatic Hydrocarbons	Benzo[ghi]perylene	Benzo(g,h,i)perylene
53-70-3	Polycyclic Aromatic Hydrocarbons	Benzo[k]tetraphene	Dibenz(a,h)anthracene
218-01-9	Polycyclic Aromatic Hydrocarbons	Chrysene	Chrysene
206-44-0	Polycyclic Aromatic Hydrocarbons	Fluoranthene	Fluoranthene

CASRN	Group	Systematic name	Synonym
193-39-5	Polycyclic Aromatic Hydrocarbons	Indeno[1,2,3-cd]pyrene	Indeno(1,2,3-cd)pyrene
91-20-3	Polycyclic Aromatic Hydrocarbons	Naphthalene	Naphthalene
85-01-8	Polycyclic Aromatic Hydrocarbons	Phenanthrene	Phenanthrene
129-00-0	Polycyclic Aromatic Hydrocarbons	Pyrene	Pyrene
56-55-3	Polycyclic Aromatic Hydrocarbons	Tetraphene	Benz(a)anthracene
7429-90-5	Trace elements	Aluminium	Al
7440-36-0	Trace elements	Antimony	Sb
7440-38-2	Trace elements	Arsenic	As
7440-42-8	Trace elements	Boron	B
7440-43-9	Trace elements	Cadmium	Cd
7440-47-3	Trace elements	Chromium	Cr
7440-48-4	Trace elements	Cobalt	Co
7440-50-8	Trace elements	Copper	Cu
7439-89-6	Trace elements	Iron	Fe
7439-92-1	Trace elements	Lead	Pb
7439-96-5	Trace elements	Manganese	Mn
7439-98-7	Trace elements	Molybdenum	Mo
7440-02-0	Trace elements	Nickel	Ni
7723-14-0	Trace elements	Phosphorus	P
7782-49-2	Trace elements	Selenium	Se
7440-21-3	Trace elements	Silicon	Si
7440-24-6	Trace elements	Strontium	Sr
7440-66-6	Trace elements	Zinc	Zn
95-14-7	Triazoles	1H-Benzotriazole (8CI, 9CI, ACI)	Benzotriazole
75-27-4	Trihalomethanes	Bromo(dichloro)methane	Bromodichloromethane
75-25-2	Trihalomethanes	Bromoform	Bromoform
67-66-3	Trihalomethanes	Chloroform	Chloroform
124-48-1	Trihalomethanes	Dibromo(chloro)methane	Dibromochloromethane
2754428-18-5	Tyre chemicals	2,5-Cyclohexadiene-1,4-dione, 2-[(1,3-dimethylbutyl)amino]-5-(phenylamino)-	6PPD Quinone
39863-30-4	Tyre chemicals	Hexamethoxymelamine	HMMM

PFAS group CASRN and systematic identifiers

CASRN	Systematic Name	Synonym
375-22-4	Perfluorobutanoic acid	PFBA
2706-90-3	Perfluoropentanoic acid	Perfluoropentanoic acid
307-24-4	Perfluorohexanoic acid	PFHxA
375-85-9	Perfluoroheptanoic acid	Perfluoroheptanoic acid
335-67-1	Perfluorooctanoic acid	PFOA
375-95-1	Perfluorononanoic acid	Perfluorononanoic acid
335-76-2	Perfluorodecanoic acid	Perfluorodecanoic acid
2058-94-8	Perfluoroundecanoic acid	Perfluoroundecanoic acid
307-55-1	Perfluorododecanoic acid	Perfluorododecanoic acid
72629-94-8	Perfluorotridecanoic acid	Perfluorotridecanoic acid
376-06-7	Perfluorotetradecanoic acid	Perfluorotetradecanoic acid
754-91-6	Perfluorooctane sulfonamide	Perfluorooctane sulfonamide
31506-32-8	*N*-Methylperfluoro-1-octane sulfonamide	*N*-Methylperfluoro-1-octane sulfonamide
4151-50-2	*N*-Ethylperfluoro-1-octane sulfonamide	*N*-Ethylperfluoro-1-octane sulfonamide
24448-09-7	2-(*N*-Methylperfluoro-1-octane sulfonamido)ethanol	2-(*N*-Methylperfluoro-1-octane sulfonamido)ethanol
1691-99-2	2-(*N*-Ethylperfluoro-1-octane sulfonamido)ethanol	2-(*N*-Ethylperfluoro-1-octane sulfonamido)ethanol
2991-50-6	*N*-Ethyl-perfluorooctanesulfonamidoacetic acid	*N*-Ethyl-perfluorooctanesulfonamidoacetic acid
2355-31-9	*N*-Methyl-perfluorooctanesulfonamidoacetic acid	*N*-Methyl-perfluorooctanesulfonamidoacetic acid
375-73-5	Perfluorobutanesulfonic acid	Perfluorobutanesulfonic acid
68259-12-1	Perfluorononane sulfonic acid	Perfluorononane sulfonic acid
423-41-6	Perfluoropropane sulfonic acid	Perfluoropropane sulfonic acid
2706-91-4	Perfluoropentane sulfonic acid	Perfluoropentane sulfonic acid
355-46-4	Perfluorohexane sulfonic acid	Perfluorohexane sulfonic acid
375-92-8	Perfluoroheptane sulfonic acid	Perfluoroheptane sulfonic acid
1763-23-1	Perfluorooctane sulfonic acid	PFOS
335-77-3	Perfluorodecane sulfonic acid	Perfluorodecane sulfonic acid
757124-72-4	1H.1H.2H.2H-Perfluorohexanesulfonic acid	1H.1H.2H.2H-Perfluorohexanesulfonic acid
27619-97-2	1H.1H.2H.2H-Perfluorooctanesulfonic acid	1H.1H.2H.2H-Perfluorooctanesulfonic acid
39108-34-4	1H.1H.2H.2H-Perfluorodecanesulfonic acid	1H.1H.2H.2H-Perfluorodecanesulfonic acid
120226-60-0	1H.1H.2H.2H-Perfluorododecanesulfonic acid	1H.1H.2H.2H-Perfluorododecanesulfonic acid

Analyte groups with no CASRN or other systematic identifiers

Group	Synonym
Bromodiphenyl Ethers	Total PBDEs
Bromodiphenyl Ethers	BDE 28 + 33
Bromodiphenyl Ethers	BDE 138 + 166
Bromodiphenyl Ethers	BDE 156 + 169
Monocyclic Aromatic Hydrocarbons	m & p-Xylenes
NEPM Total Recoverable Hydrocarbons	TRH C6 - C10
NEPM Total Recoverable Hydrocarbons	TRH C6 - C10 less BTEX(F1)
NEPM Total Recoverable Hydrocarbons	TRH>C10 - C16
NEPM Total Recoverable Hydrocarbons	TRH>C10 - C16 less Naph(F2)
NEPM Total Recoverable Hydrocarbons	TRH>C16 - C34(F3)
NEPM Total Recoverable Hydrocarbons	TRH>C34 - C40(F4)
Phenols	3&4-Methylphenol
Polychlorinated biphenyl	Total PCB
Polycyclic Aromatic Hydrocarbons	Benzo(b,k)fluoranthene
Solution	E.C.
Solution	pH
Total Recoverable Hydrocarbons (formerly TPH)	TRH C6 - C9
Total Recoverable Hydrocarbons (formerly TPH)	TRH C10 - C14
Total Recoverable Hydrocarbons (formerly TPH)	TRH C15 - C28
Total Recoverable Hydrocarbons (formerly TPH)	TRH C29 - C36
Triazoles	Tolyltriazole (4-methylbenzotriazole & 5-methylbenzotriazole)*