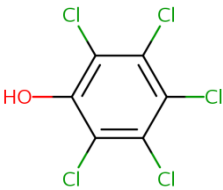
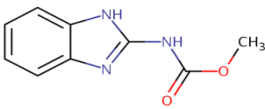
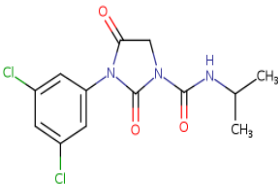
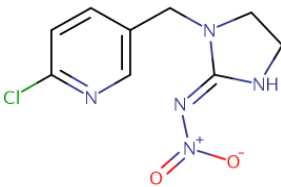
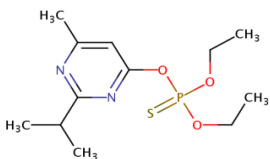
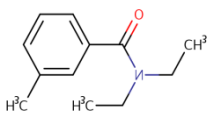
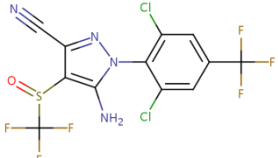
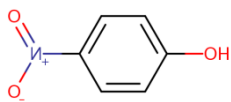
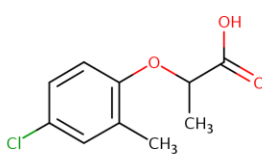
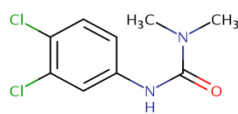


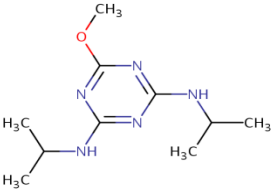
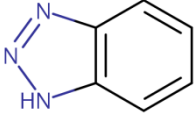
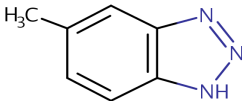
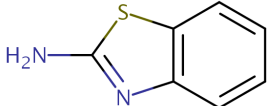
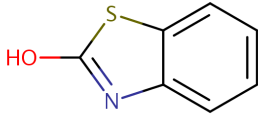
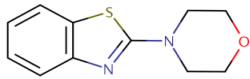
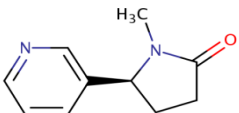
Targeted method description:

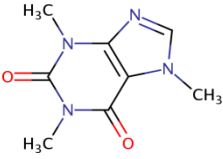
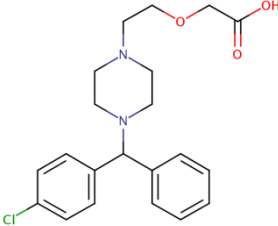
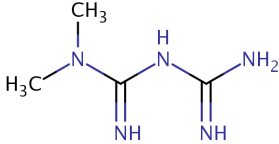
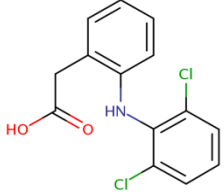
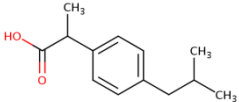
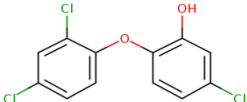
Urban stormwater runoff is a major carrier of chemical contaminants into receiving waters, resulting in water quality degradation. There is growing awareness of the potential toxicological relevance of organic contaminants in the aquatic environment. Our goal was to select a suite of representative tracers for urban runoff that includes a broad range of contaminants with different physical-chemical parameters (e.g, various chemical functionalities, wide range of polarities and biodegradation potential). The compounds were selected to represent 3 primary urban sources: residential use, roadways, and wastewater. We developed a targeted analytical method to assess analyte concentrations, using multi-residue solid phase extraction (SPE) and liquid chromatography with tandem mass spectroscopy (LC-MS/MS) to analyze more than 35 compounds including pharmaceuticals, pesticides, and several vehicle-specific analytes. The target compounds are listed in Table 1.

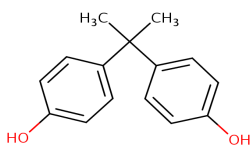
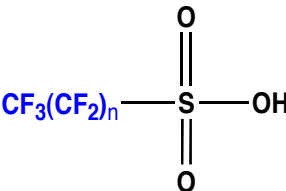
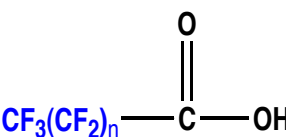
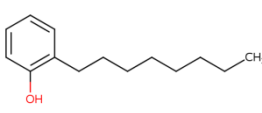
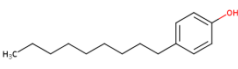
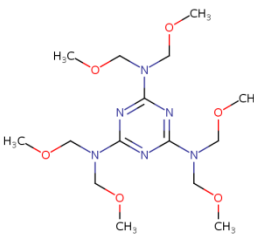
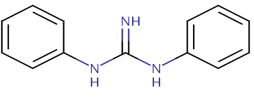
Table 1. Proposed target analytes for water quality characterization of urban stormwater via LC-MS/MS.

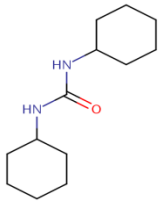
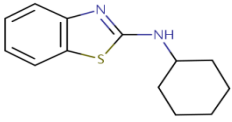
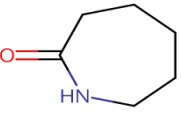
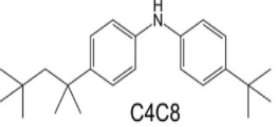
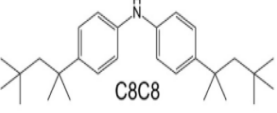
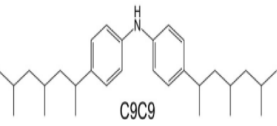
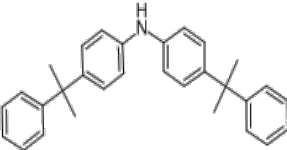
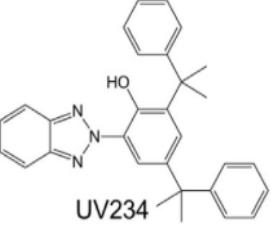
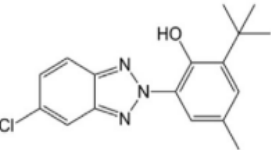
Compound	Category	Structure	Sources
Pentachlorophenol	Fungicide		Recreational, Industrial, Road (eg. utility poles, railroad ties)
Carbendazim	Fungicide		Residential (new antifouling paints and renders, biocidal compounds in roof paints)
Iprodione	Fungicide		Residential
Imidacloprid	Pesticide		Residential (main neonic in use in urban areas)

Diazinon	Insecticide		Residential (on lawns and gardens)
DEET	Insecticide		Residential (insect repellent) *More from WW than from residential surface runoff
Fipronil	Insecticide		Residential (southern>northern)
4-Nitrophenol	Insecticide (Transformation Product)		Residential
Mecoprop	Herbicide		Recreational (yards, parks, railway mainten)
Diuron	Herbicide		Residential, Recreational, Road (building facade paints and renders, for yards, parks, and railway maintenance)

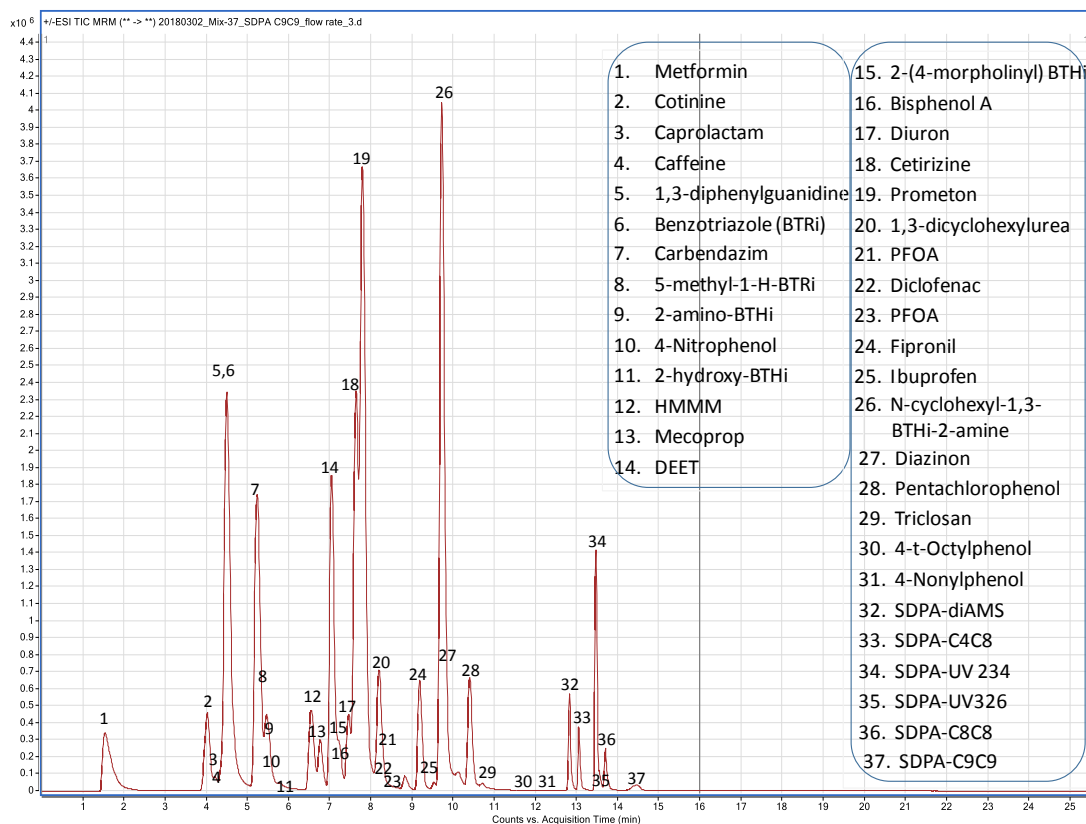
Prometon	Herbicide		Residential (homeowner use); Road
Benzotriazole	Benzotriazole		Wastewater & stormwater Industrial (antifreezer formulation, cooling system);
5-methyl-1H-benzotriazole	Benzotriazole		Residential (dishwasher detergent). Highway Road (tire particles, used as marker of tire rubber)
2-amino-benzothiazole	Benzothiazole		
2-hydroxy-benzothiazole	Benzothiazole		
2-(4-morpholinyl)benzothiazole (2,4-MoBT)	Benzothiazole		
Cotinine	Pharmaceutical – Stimulant		Wastewater & stormwater

Caffeine	Pharmaceutical – Stimulant		Wastewater & stormwater
Cetirizine	Pharmaceutical – Antihistamine		Wastewater & stormwater
Metformin	Pharmaceutical – Endocrine-active compound		Wastewater
Diclofenac	Pharmaceutical – Anti-inflammatory		Wastewater
Ibuprofen	Pharmaceutical – Analgesic		Wastewater
Triclosan	Pharmaceutical – Antibacterial and disinfectant		Wastewater

Bisphenol A	Pharmaceutical		*Ubiquitous in the environment (as surface treatment agents, polymers, metal coating, and fire retardants)
PFOS (Perfluorooctanesulfonic acid) (n=7)	PFAs		
PFOA (n=6)	PFAs		
4-Octylphenol (OP)	Surfactant and surfactant metabolites		Road (asphalt, vehicle parts)
4-Nonylphenol (NP)	Surfactant and surfactant metabolites		Residential/Industrial (surfactant or emulsifier in paints, concrete, building materials, detergent and cosmetic products, etc.)
Hexa(methoxymethyl)melamine (HMMM)	Vehicle-specific analytes		Tire and road wear particles (TRWP)
1,3-diphenylguanidine	Vehicle-specific analytes		Tire and road wear particles (TRWP)

1,3-dicyclohexylurea	Vehicle-specific analytes		Tire and road wear particles (TRWP)
N-cyclohexyl-1,3-benzothiazol-2-amine	Vehicle-specific analytes		Tire and road wear particles (TRWP)
Caprolactam	Stormwater (Lee Ferguson)		Ubiquitous Industrial (used in the manufacture of Nylon-6)
C4C8	SDPA/UV stabilizers		Wastewater & stormwater (**these were selected from larger group based on occurrence in environment (Lu et al_Envi. Canada))
C8C8	SDPA/UV stabilizers		
C9C9	SDPA/UV stabilizers		
diAMS	SDPA/UV stabilizers		
UV-234	SDPA/UV stabilizers		
UV326	SDPA/UV stabilizers		

LC Chromatogram and Targeted Analyte List for Urban Stormwaters.



Key detections commonly observed in Puget Sound stormwater/surface water via suspect screening with high resolution mass spectrometry. There is significant overlap with the method above as we built the LC/MS/MS method from the HRMS data:

- HMMM family: Hexa(methoxymethyl)melamine, di-formylated HMMM, hexamethylolmelamine pentamethyl ether, tetra(methoxymethyl)melamine, penta(methoxymethyl)melamine
- 1,3-dicyclohexylurea
- 1,3-diphenylguanidine
- 1-cyclohexyl-3-phenylurea
- Dicyclohexylamine
- 4(5)-methylbenzotriazole
- DEET
- Diuron
- Cotinine
- Tris(2-chloropropyl)phosphate
- Tris(2-butoxyethyl)phosphate
- Many series of polyethylene glycols and polypropylene glycols