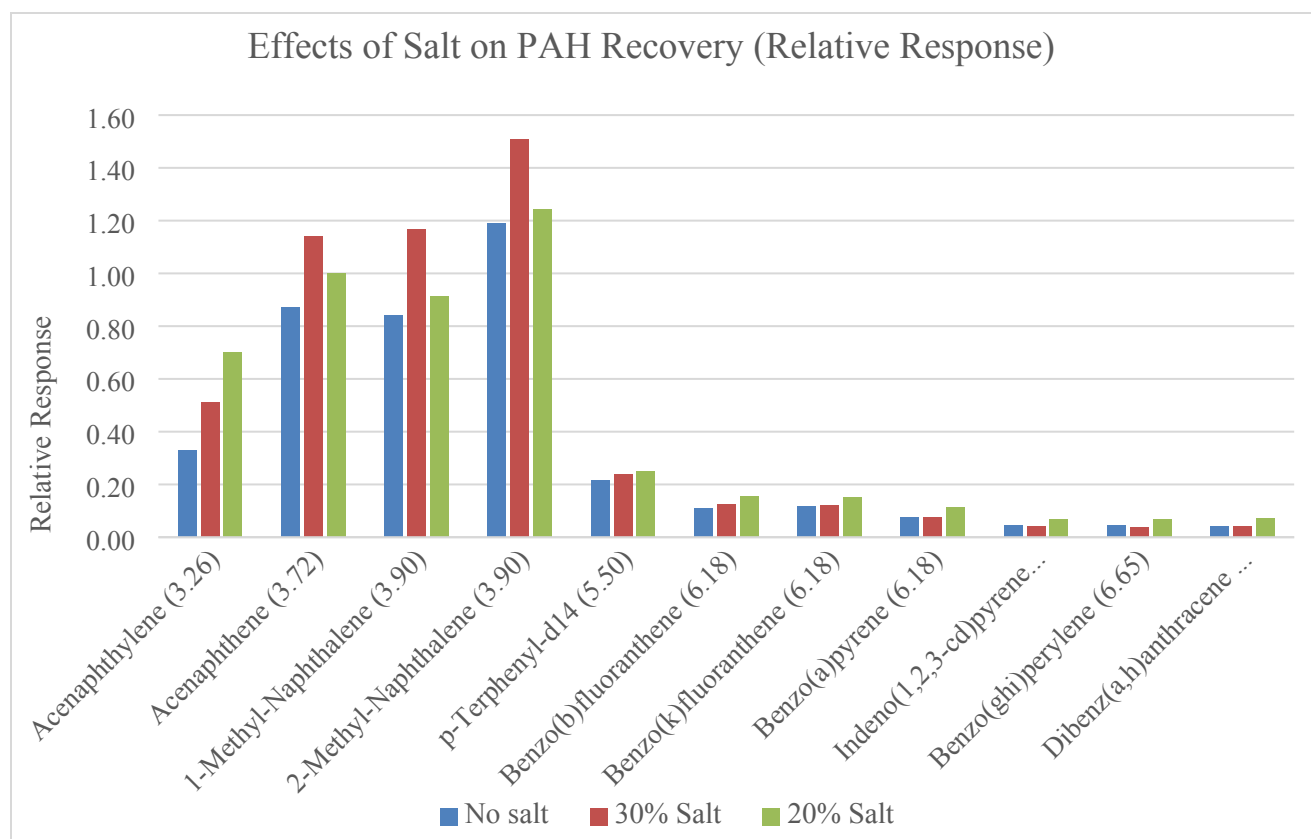


**Supplemental Information for A Suspect Screening Analysis for Contaminants of  
Emerging Concern in Municipal Wastewater and Surface Water Using Liquid-Liquid  
Extraction and Stir Bar Sorptive Extraction.**

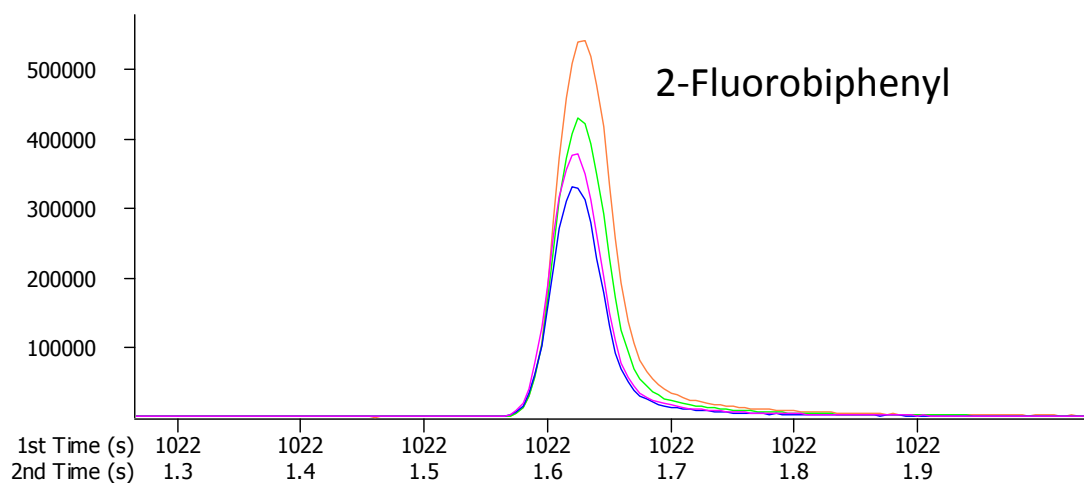
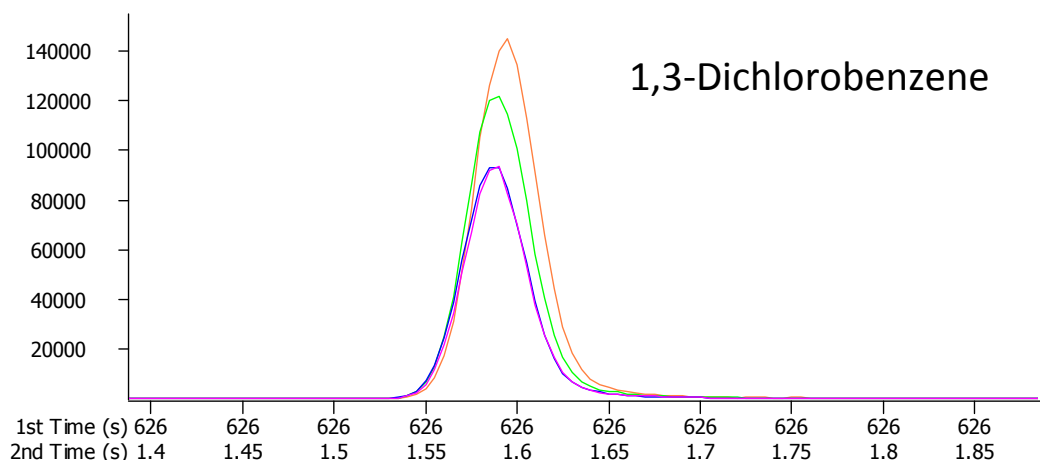
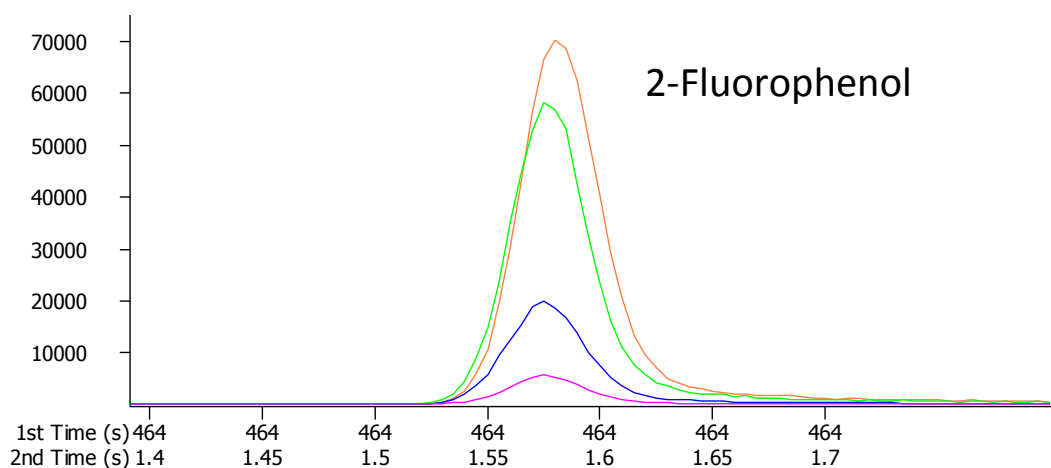
**Additional Materials and Methods Information:**

All the analytical standards, including surrogates, calibration mix, internal standards and hexachlorobenzene (cat # 32231) were purchased from Restek Corp. (Bellefonte, PA, USA). The surrogate standards include the Acid Surrogate Standard Mix (cat # 31003), Base Neutral Surrogate Standard Mix (cat # 31082) and QuEChERS Internal Standard Mix for GC-MS Analysis (cat # 33267). These were chosen because they represent environmentally relevant compound classes and provide a range of acidic and basic compounds. SV Internal Standard Mix (cat # 31206), a solution of 6 deuterated polycyclic aromatic hydrocarbons, was used because of its compliance with the US EPA Method 8270D for analysis of semi-volatile organic pollutants by GC-MS. 8270 Megamix (cat# 31850) was utilized as an additional calibration and target mix of 76 common environmental pollutants. Any sample analytes found in 8270 Megamix could then be quantified and it could also serve for single point semi-quantification purposes.

Analytical grade dichloromethane, methanol and acetonitrile were purchased from Avantor (Center Valley, PA, USA), ChemPure Brand Chemicals (Ann Arbor, MI, USA) and Avantor respectively. The sodium sulfate and sodium chloride were supplied by Avantor and VWR (West Chester, PA, USA). The ultrapure water was delivered by the lab system Millipore Milli-Q Academic Ultrapure Water System (Billerica, MA, USA).



**Figure S1:** Graph showing the relative response of PAHs as a function of the NaCl concentration during extraction. The logKow values are in parenthesis next to the analyte name.



**Figure S2:** Extracted Ion Chromatograms showing the CIS trapping temperature effects on peak area. Orange represents -100 °C, green is -80 °C, blue is -50 °C, and pink is -20 °C.

**Table S.1.** Percent Recoveries of sample method blanks

	Compound	LLE WW Method Blank	LLE Spring Creek Method Blank	SBSE WW Method Blank	SBSE Spring Creek Method Blank
		%R	%R	%R	%R
Acid Surrogate Standard Mix (3/90 SOW)	2-Fluorophenol	53	29	ND	ND
	Phenol-d6	20	ND	ND	ND
	2-Chlorophenol-d-4	66	56	ND	ND
	2,4,6-Tribromophenol	28	88	ND	ND
Base Neutral Surrogate Standard Mix (3/90 SOW)	1,2- Dichlorobenzene-d4	62	145	82	109
	2-Fluorobiphenyl	53	66	81	95
	Nitrobenzene-d5	63	94	47	ND
	p-Terphenyl-d14	80	113	73	100
QuEChERS Internal Standard Mix for GC-MS Analysis	PCB 18 = 1,1'-Biphenyl, 2,2',5-trichloro-	80	99	100	127
	PCB 28 =1,1'-Biphenyl, 2,4,4'-trichloro-	80	109	85	114
	PCB 52 =1,1'-Biphenyl, 2,2',5,5'-tetrachloro-	87	93	97	121
	Triphenylmethane	93	95	88	123
	Triphenylphosphate	88	68	NLR	NLR
	Tris-(1,3-dichloro isopropyl)phosphate	92	70	NLR	NLR

LLE samples (n=2), SBSE (n=1). ND, non-detected. NLR, non-linear response.

US EPA Comptox Chemistry Dashboard lists searched:

EPA|ENDOCRINE: Endocrine Disruptor Screening Program (EDSP) Universe of Chemicals  
WATER|NORMAN: French Monitoring List

DRUGS|NORMAN: Pharmaceutical List with EU, Swiss, US Consumption Data  
 WATER|NORMAN: Wastewater Suspect List based on Swedish Product Data  
 PESTICIDES|EPA: Pesticide Chemical Search Database

**Table S.2.** Discovery compounds from the wastewater and spring creek samples.

Compound	Similarity	Reverse	Type
2-Butanol	816	957	PCP-flavorant, fragrance
Dimenhydrinate	939	939	Drug-antiemetic
Lidocaine	904	904	Drug-anesthetic
Diphenyl sulfone	936	936	Manufacturing-colorant
Doxepin	952	952	Drug-antidepressant
2-(methylthio)-benzothiazole	955	958	Consumer product
Crotamiton	933	933	Drug-antiparasitic
Amitriptyline	971	971	Drug-antidepressant
Venlafaxine	943	947	Drug-antidepressant
3,4-Dichloro-benzenamine	953	955	Herbicide precursor
Tramadol	866	866	Drug-analgesic
Citalopram	915	915	Drug-antidepressant
Bupropion	899	904	Drug-antidepressant
Methadone	917	917	Drug-opioid
Maltol	952	955	PCP-flavorant
Musk ketone	932	941	PCP- fragrance
Propofol	927	929	Drug-anesthetic
Triclosan	878	896	PCP-Antibacterial
Oxybenzone	896	896	PCP-sunscreen
Levomenthol	957	957	Drug-anesthetic
Thymol	742	771	PCP-Antibacterial
Benzophenone	952	952	PCP-sunscreen
Eucalyptol	933	933	PCP-fragrance
Butylated Hydroxytoluene	889	890	PCP- body wash, makeup
Benzothiazole	926	945	PCP-fragrance
Cedrol	861	862	PCP- emollient
Caffeine	952	952	PCP-eye cream, stimulant
Homosalate	917	922	PCP-sunscreen
Benadryl	911	928	Drug-antihistamine
Carbamazepine	805	860	Drug-anticonvulsant
Ibuprofen	791	856	Drug-analgesic
Atrazine	845	846	Pesticide

PCP, personal care product. Consumer product is the label on the EPA Comptox Database when the descriptor is not clear about the use. Similarity-number from the NIST search algorithm that defines how well the peak matches the library match using all masses, between 0-999. Reverse-

number from NIST search algorithm defines how well the peak matches the library using masses in the database, between 0-999.<sup>1</sup>

1 Leco Corporation, *ChromaTOF® Software Instruction Manual*, 2012.