Supporting information

Aquatic exposures of chemical mixtures in urban environments: approaches to impact assessment

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Table S-X1 Quantitative measurements of concentrations in runoff, ranked according to predicted toxic impact as calculated on the basis of toxic units (TU = Concentration/Average EC_{50} over species)

Origin	Contaminant group	Contaminant	Pseudo Mode of Action	Concentration 90% [µg/L]	Geometric Avg EC_{50} (µg/L)	Toxic pressure (PAF)	Toxic Units (TU)	% of ΣTU	Reference
Brake pads, roofing	Metal	Copper (dissolved)	Cu	33	183	20%	0.18	37.6%	[1]
Garden, park, building	Insecticide	Deltamethrin	Pyrethrin	0.084	2	13.7%	0.04	9.0%	[2]
Garden, park, building	Insecticide	Bifenthrin	Pyrethrin	0.030	1	11.4%	0.03	6.5%	[3]
Garden, park, building	Insecticide	Permethrin	Pyrethrin	0.202	12	7.8%	0.02	3.5%	[2]
Galvanized metal structures	Metal	Zinc (dissolved)	Zn	84.	1903	7%	0.04	9.2%	[2]
Combustion	PAH	Benz(a)anthracene	Non polar narcosis	0.192	10	0.7%	0.02	4.0%	[2]
Metal structures	Metal	Aluminum (reactive)	All	24.2	1925	0.5%	0.01	2.6%	[1]
Metal structures	Metal	Iron (dissolved)	Fe	1106	66298	0.4%	0.02	3.5%	[1]
Sewage, buildings, surfactants	Plasticiser	Nonylphenol 1 ethoxylate (NP1EO)	Non polar narcosis	4.165	525	0.1%	0.01	1.7%	[1]
Combustion	PAH	Fluoranthene	Non polar narcosis	0.887	136	0.1%	0.01	1.4%	[2]
Sewage, garden	Nutrient	Total phosphorus (as P)	P	1.800	3540	1.8%	0.001	0.1%	[1]
Industrial	Metal	Silver (dissolved)	Silver	0.250	198	0.8%	0.00	0.3%	[2]
Garden, park, building	Insecticide	Esfenvalerate	Pyrethrin	0.001	1	0.8%	0.00	0.2%	[2]
Antifouling	Organotin	Tributyltin	Multi site inhibition	0.004	2	0.5%	0.00	0.4%	[4]
Garden, pavement	Herbicide	Glyphosate	Organophosphate	67.5	42501	0.5%	0.00	0.3%	[1]
Garden, park, building	Insecticide	Fipronil	Pyrazole	0.05	24	0.4%	0.00	0.4%	[3]
Sewage	Pharmaceutical	Ibuprofen	Analgesics	1.489	19738	0.3%	0.00	0.0%	[4]
Roofing	Metal	Lead (dissolved)	Pb	17.2	5298	0.2%	0.00	0.7%	[1]
Industrial	Metal	Nickel (dissolved)	Ni	5	2659	0.2%	0.00	0.4%	[1]

Origin	Contaminant group	Contaminant	Pseudo Mode of Action	Concentration 90% [µg/L]	Geometric Avg EC_{50} (µg/L)	Toxic pressure (PAF)	Toxic Units (TU)	% of ΣTU	Reference
Industrial	Metal	Cadmium (dissolved)	Cd	0.372	862	0.2%	0.00	0.1%	[4]
Legacy insecticide	Insecticide	DDT(p,p')	Organochlorine	0.009	25	0.1%	0.00	0.1%	[2]
Industrial	Metal	Tin (dissolved)	Sn	0.84	3439	0.1%	0.00	0.1%	[2]
Plastic building materials	Plasticiser	Nonylphenol	Non polar narcosis	2.48	525	0.0%	0.00	1.0%	[1]
Sewage	Chelator	Ethylenediaminetetraacetic acid (EDTA)	Chelation	434	95763	0.0%	0.00	0.9%	[4]
Sewage	Biocide	Triclosan	Biocide	0.514	122	0.0%	0.00	0.9%	[1] [4]
Combustion	PAH	Pyrene	Non polar narcosis	0.632	174	0.0%	0.00	0.8%	[2]
Industrial	Metal	Vanadium (dissolved)	Va	3.7	1104	0.0%	0.00	0.7%	[2]
Combustion	PAH	Benzo(e)pyrene	Non polar narcosis	0.313	172	0.0%	0.00	0.4%	[2]
Combustion	PAH	Benzo(g,h,i)perylene	Non polar narcosis	0.299	172	0.0%	0.00	0.4%	[2]
Combustion	PAH	Perylene	Non polar narcosis	0.298	172	0.0%	0.00	0.4%	[2]
Plastic building materials	Plasticiser	Diethylhexylphthalate	Diester toxicity	5.16	3538	0.0%	0.00	0.3%	[1]
Plastic building materials	Plasticiser	Bisphenol-A	Polar Narcosis	3.16	3261	0.0%	0.00	0.2%	[1]
Combustion	PAH	Benzo(k)fluoranthene	non polar narcosis	0.154	172	0.0%	0.00	0.2%	[2]
Legacy industrial	PCB	PCB66	PCB	0.024	28	0.0%	0.00	0.2%	[2]
Legacy industrial	PCB	PCB52	PCB	0.022	28	0.0%	0.00	0.2%	[2]
Wood preservative	Metal	Arsenic (dissolved)	As	2	2479	0.0%	0.00	0.2%	[2]
Industrial	Metal	Strontium (dissolved)	Sr	102	127938	0.0%	0.00	0.2%	[2]

Origin	Contaminant group	Contaminant	Pseudo Mode of Action	Concentration 90% [µg/L]	Geometric Avg EC_{50} (µg/L)	Toxic pressure (PAF)	Toxic Units (TU)	% of ΣTU	Reference
Combustion	PAH	Naphthalene	Non polar narcosis	2.66	4146	0.0%	0.00	0.1%	[1]
Legacy industrial	PCB	PCB95	PCB	0.016	28	0.0%	0.00	0.1%	[2]
Combustion	PAH	Benzo(a)pyrene	Non polar narcosis	0.094	172	0.0%	0.00	0.1%	[4]
Legacy industrial	PCB	PCB110	PCB	0.015	28	0.0%	0.00	0.1%	[2]
Combustion	PAH	Benzo(b)fluoranthene	Non polar narcosis	0.533	1024	0.0%	0.00	0.1%	[2]
Legacy industrial	PCB	PCB49	PCB	0.013	28	0.0%	0.00	0.1%	[2]
Legacy industrial	PCB	PCB44	PCB	0.013	28	0.0%	0.00	0.1%	[2]
Legacy industrial	PCB	PCB31	PCB	0.012	28	0.0%	0.00	0.1%	[2]
Garden, pavement	Herbicide	Bentazone	Unclassified herbicides	50	133137	0.0%	0.00	0.1%	[1]
Legacy industrial	PCB	PCB101	PCB	0.01	28	0.0%	0.00	0.1%	[2]
Legacy insecticide	Insecticide	DDD(p,p')	Organochlorine	0.006	20	0.0%	0.00	0.1%	[2]
Combustion	PAH	Chrysene	Non polar narcosis	0.315	1264	0.0%	0.00	0.1%	[2]
Legacy insecticide	Insecticide	DDT(o,p')	Organochlorine	0.005	25	0.0%	0.00	0.0%	[2]
Industrial	Metal	Antimony (dissolved)	Sb	2.2	10421	0.0%	0.00	0.0%	[2]
Legacy insecticide	Insecticide	DDE(p,p')	Organochlorine	0.016	84	0.0%	0.00	0.0%	[2]
Garden, pavement	Herbicide	Mecoprop	Phenoxypropanoic	5	31835	0.0%	0.00	0.0%	[1]
Garden, park, building	Insecticide	Carbaryl	Carbamate	0.08	731	0.0%	0.00	0.0%	[3]
Combustion	PAH	Dibenz(a,h)anthracene	Non polar narcosis	0.053	496	0.0%	0.00	0.0%	[2]
Garden, pavement	Herbicide	Diuron	Phenylurea	0.07	673	0.0%	0.00	0.0%	[3]
Combustion	PAH	Dibenzothiophene	Non polar narcosis	0.064	638	0.0%	0.00	0.0%	[2]
Industrial	Metal	Barium (dissolved)	Ba	16	227248	0.0%	0.00	0.0%	[2]
Garden, pavement	Herbicide	Triclopyr	Pyridine	0.22	3595	0.0%	0.00	0.0%	[3]
Garden, park, building	Insecticide	Fipronilsulfone	Pyrazole	0.01	164	0.0%	0.00	0.0%	[3]

Origin	Contaminant group	Contaminant	Pseudo Mode of Action	Concentration 90% [µg/L]	Geometric Avg EC_{50} (µg/L)	Toxic pressure (PAF)	Toxic Units (TU)	% of ΣTU	Reference
Industrial	Metal	Selenium (dissolved)	Se	0.4	8855	0.0%	0.00	0.0%	[2]
Legacy insecticide	Insecticide	DDE(o,p')	Organochlorine	0.003	84	0.0%	0.00	0.0%	[2]
Garden, park, building	Insecticide	Dichlorvos	Organophosphate	0.01	334	0.0%	0.00	0.0%	[3]
Garden, pavement	Herbicide	2,4-D	Phenoxyacetic	1.2	50992	0.0%	0.00	0.0%	[3]
Sewage	Pharmaceutical	Oxytetracycline	Bactericide	0.496	21948	0.0%	0.00	0.0%	[4]
Sewage	Pharmaceutical	Diclofenac	Analgesics	0.422	26388	0.0%	0.00	0.0%	[4]
Sewage	Pharmaceutical	Erythromycin	Bactericide	0.124	15406	0.0%	0.00	0.0%	[4]
Sewage	Pharmaceutical	Fluoxetine	Antidepressant	0.042	6039	0.0%	0.00	0.0%	[4]
Garden, pavement	Herbicide	Dicamba	Benzoic acid	0.17	26971	0.0%	0.00	0.0%	[3]
Sewage	Estrogen	Estrone (E1)	Estrogenic	0.007	1269	0.0%	0.00	0.0%	[4]
Sewage	Pharmaceutical	Propranolol	Cardiovascular	0.025	4347	0.0%	0.00	0.0%	[4]
Sewage	Pharmaceutical	Ofloxacin	Bactericide	0.025	6688	0.0%	0.00	0.0%	[4]
Sewage	Estrogen	Estradiol (E2)	Estrogenic	0.004	1269	0.0%	0.00	0.0%	[4]
Industrial	Metal	Beryllium (dissolved)	Be	0.100	32382	0.0%	0.00	0.0%	[2]
Garden, pavement	Herbicide	2-methyl-4-chlorophenoxyacetic acid (MCPA)	Phenoxy-acetic	0.070	29100	0.0%	0.00	0.0%	[3](
Garden, pavement	Herbicide	Prometon	Methoxy-triazine	0.060	28510	0.0%	0.00	0.0%	[3]
Sewage	Estrogen	Ethinyl estradiol (EE2)	Estrogenic	0.001	1865	0.0%	0.00	0.0%	[4]
						msPAF mixed model = 49.6%	ΣTU = 0.43	Sum %TU = 100%	

Table S-X2 Potential information sources for obtaining emission data for chemicals in construction materials used in the urban environment

Source	Substance	Category	Description	Release factor	Unit	Reference
REACH TG	not specified	ERC10a	Wide dispersive outdoor use of long-life articles and materials with low release. Default worst case release factor	3.2	% to water (before STP)	[5]
REACH TG	not specified	ERC10b	Wide dispersive outdoor use of long-life articles and materials with high or in-tended release (including abrasive processing). Default worst case release factor	100	% to water (before STP)	[5]
Building and construction products	medium-chain chlorinated paraffins (MCCPs)			0.0325	to water, kg/kg MCCP in product (3.25%)	[6]
concrete and plaster	Nonyl phenol ethoxylates (NPEs)			0.2	mg/m2 annual release factor to strom water per surface area of construction	[6]
insulating material	Brominated flame retardants (BFRs)			0.70	% outdoor use, to water percentage is annual worst case factor to the amount of BFR in the product	[6]
roofing, flashings and other exterior structures	lead	Lead sheets	5g/m2(corrosion rate) for lead sheet, implies emission factor of 0.008-0.01% annual, taking into acount estimated total stock of lead sheet used for buildings in Netherland. Assuming 75% of runoff ends up to soil. This implies rest 25% to water as worst case	0.002	% for water	[6]
roofing, flashings and other exterior structures	Bis(2-ethylhexyl) phthalate (DEHP)	roofing material		0.985 2.31	g/m2 (clean surface), annual g/m2 (unclean surface), annual water and soil (seems total)	[6]
wall and floor coverings	hard plastics	NPs/NPEs		2.78*E-12	kg/m2 used amount of plastics annually, to storm water	[6]

Source	Substance	Category	Description	Release factor	Unit	Reference
wall and floor coverings	soft plastics	NPs/NPEs		4.64*E-12 kg/m2 used amount of plastics annually	kg/m2 used amount of plastics annually, to storm water	[6]
surface coatings and adhesives	antifoulings	copper, TBT		0.81	kg/kg/ paint used, to water	[6]

Table S-X3 List of water pollutants included in the European Pollutant Release and Transfer Register (EPRTR). Specific requirements for emissions reporting depend on industry sector and emission limits [7].

Substance / Parameter	Reporting Limit (kg/y)	Substance / Parameter	Reporting Limit (kg/y)
Nutrients		***Halogenated compounds***	
Total nitrogen	50 000	1,2-dichloroethane	10
Total phosphorus	5 000	Brominated diphenylethers	1
Total organic carbon or COD	50000	Chloro-alkanes, C10-C13	1
Metals		Dichloromethane	10
Arsenic	5	Hexabromobiphenyl	0.1
Cadmium	5	Hexachlorobenzene	1
Chromium	50	Hexachlorobutadiene	1
Copper	50	PCDD + PCDF (dioxins + furans)	0.0001*
Mercury	1	Pentachlorobenzene	1
Nickel	20	Pentachlorophenol	1
Lead	20	Polychlorinated biphenyls	0.1
Zinc	100	Tetrachloroethylene	10
Inorganics		Tetrachloromethane	1
Chlorides (as total Cl)	2.00E+06	Trichlorobenzenes	1
Asbestos	1	Trichloroethylene	10
Cyanides (as total CN)	50	Trichloromethane	10
Fluorides (as total F)	2000	Vinyl chloride	10
Hydrocarbons		***Pesticides***	
Anthracene	1	1,2,3,4,5,6-hexachlorocyclohexane	1
Benzene	200**	Alachlor	1
Ethyl benzene	200**	Aldrin	1
Naphthalene	10	Atrazine	1
Polycyclic aromatic hydrocarbons	5***	Chlordane	1
Toluene	200*	Chlordecone	1
Xylenes	200**	Chlorfenvinphos	1
Fluoranthene	1	Chlorpyrifos	1
Benzo(g,h,i)perylene	1	DDT	1
Phenols/Ethoxylates		Dieldrin	1
Phenols (as total C)	20	Diuron	1
Nonylphenol and ethoxylates	1	Endosulphan	1

Substance / Parameter	Reporting Limit (kg/y)	Substance / Parameter	Reporting Limit (kg/y)
Octylphenols and ethoxylates	1	Endrin	1
Organometalics		Heptachlor	1
Organotin (total Sn)	50	Isodrin	1
Tributyltin and compounds	1	Isoproturon	1
Triphenyltin and compounds	1	Lindane	1
Other organic chemicals		Mirex	1
Di-(2-ethyl hexyl) phthalate	1	Simazine	1
Ethylene oxide	10	Toxaphene	1
Halogenated organic compounds	1000	Trifluralin	1

* as Toxic Equivalents (i.e. TEQ)

** single substances are to be reported if the threshold for BTEX (the sum parameter of benzene, toluene, ethyl benzene, xylenes) is exceeded

*** fluoranthene, benzo[*b*]fluoranthene, benzo[*a*]pyrene, benzo[*k*]fluoranthene, indeno[1,2,3-*cd*]pyrene, and benzo[*ghi*]perylene.

Table S-X4. Assessment of TU for the chemical and paper/wood processing sectors using the 2012 EPRTR emission inventory

Substance		Sector Chemicals			Sector Paper & Wood Processing		
Substance	**Avg EC_{50} µg/L**	**Emission to Water (kg/y)**	**Toxicity Normalized Emission**	**% Contribution to TUs**	**Emission to Water (kg/y)**	**Toxicity Normalized Emission**	**% Contribution to Tus**
chlorinated organics							
1,2-dichloroethane	165959	3780	2.28E-02	0.00			
Dichloromethane	199526	4680	2.35E-02	0.00			
Hexachlorobenzene	708	2.5	3.53E-03	0.00			
Hexachlorobutadiene	407	158	3.88E-01	0.00			
Pentachlorobenzene	550	44	8.01E-02	0.00			
Pentachlorophenol	417	8.76	2.10E-02	0.00	5.9	1.42E-02	0.00
Tetrachloroethylene	15488	933	6.02E-02	0.00			
Tetrachloromethane	39811	916	2.30E-02	0.00			
Trichlorobenzenes	2512	297	1.18E-01	0.00			
Trichloroethylene	57544	720	1.25E-02	0.00	98.8	1.72E-03	0.00
Trichloromethane	74131	4533	6.11E-02	0.00	132	1.78E-03	0.00
Metals							
Arsenic	2399	8431	3.51E+00	0.00	2310	9.63E-01	0.00
Cadmium	794	3586.3	4.51E+00	0.00	1060	1.33E+00	0.00
Chromium	7079	31009	4.38E+00	0.00	4840	6.84E-01	0.00
Copper	162	18003.6	1.11E+02	0.00	17700	1.09E+02	0.32
Mercury	240	735	3.06E+00	0.00	96.1	4.01E-01	0.00
Nickel	4898	25831	5.27E+00	0.00	7180	1.47E+00	0.00
Lead	5248	11400	2.17E+00	0.00	2570	4.90E-01	0.00
Zinc	1862	139095	7.47E+01	0.00	128000	6.87E+01	0.20
Inorganics							
Chlorides (as total Cl)	3020	9424530000	3.12E+06	96.76	102120000	3.38E+04	98.52
	4074	13900	3.41E+00	0.00	6590	1.62E+00	0.00
	48	4953299	1.03E+05	3.21	6730	1.41E+02	0.41

Substance		Sector Chemicals			Sector Paper & Wood Processing		
Substance	Avg EC_{50} µg/L	Emission to Water (kg/y)	Toxicity Normalized Emission	% Contribution to TUs	Emission to Water (kg/y)	Toxicity Normalized Emission	% Contribution to Tus
Ammonia (est. from Total N)	6918.31	4707800	6.80E+02	0.02	1207600	1.75E+02	0.51
Total P	4897788	823810	1.68E-01	0.00	766000	1.56E-01	0.00
Hydrocarbons							
Anthracene	19	1.9	9.74E-02	0.00			
Benzene	101373	4230	4.17E-02	0.00			
Ethyl benzene	13725	1730	1.26E-01	0.00			
Naphthalene	4929	244	4.95E-02	0.00			
Toluene	31029	7640	2.46E-01	0.00	176000	5.67E+00	0.02
Xylenes	11786	20.1	1.71E-03	0.00			
Fluoranthene	191	8.1	4.25E-02	0.00			
Phenols/Ethoxylates/Plasticizers							
Phenols (as total C)	108961	52900	4.85E-01	0.00	16900	1.55E-01	0.00
Nonylphenol and ethoxylates	603	1192	1.98E+00	0.00	959	1.59E+00	0.00
Octylphenols and ethoxylates	400	684	1.71E+00	0.00	6.4	1.60E-02	0.00
Di-2-ethylhexyl phthalate	3548	135	3.80E-02	0.00	135	3.80E-02	0.00
Pesticides							
1,2,3,4,5,6-hexachlorocyclohexane	186	37.2	2.00E-01				
Aldrin	60				2.7		0.00
Atrazine	2188				1.06		0.00
Dieldrin	61				2.7		0.00
Diuron	1259	2.71	2.15E-03				
Endrin	3				1.4		0.00
Isodrin	9				1.4		0.00
Simazine	14125				1.06		0.00
			3.23E+06	100.0		3.43E+04	100.0

Table S-X5 Contaminant Profile for European Refinery Effluents [8]

Substance	Median (µg/L)	90th % ile (µg/L)	Substance	Median (µg/L)	90th % ile (µg/L)
Metals			***Organics***		
Arsenic	11	20	Benzene	2.7	232
Cadmium	21	36	Toluene	5.3	158
Chromium	11	35	Ethylbenzene	3.2	16
Cobalt	3	20	Xylenes	20	182
Copper	9	17	Naphthalene	4.3	320
Mercury	0.1	0.5	1,2 dichlorethane	1.6	113
Lead	12	12	1,2 dichloroethene	22	38
Nickel	11	26	trichlorethane	0.35	1.93
Vandium	9	35	trichloroethene	15	27
Zinc	45	110	tetrachloroethene	0.5	24

Appendix text S1.

An example of European EPTR query that describes wastewater emissions form an urban sewage treatment works treating industrial waste waters

Blackburn is a town in Lancashire, England located 14 km east of Preston and 20.9 miles of northwest Manchester. Blackburn represents an urban area with a long history of industrialization with a population, including the nearby town of Darwen, of over 147,000 in 2013 [9]. Chemical pollution from the water treatment industry and urban related sources, as well as physical habitat modifications, have been identified as the dominant causes for use impairment for the River Darwen that flows through this region [10].

A query of the on-line European PRTR indicates that there are 15 industries in Blackburn and 5 in Darwen. The sectors and number of facilities in each sector are: Energy (1 facility); Production and processing of metal ores (1); Chemicals Industry (4); Waste and wastewater management (9); Animal and vegetable products from the food and beverage sector (2); and Other miscellaneous activities (3). None of these facilities report direct releases of wastewater to local receiving water but most report wastewater transfers. A major recipient of these industrial wastewaters appears to be the Blackburn sewage treatment works which has been in operation since the 19th century. This facility treats domestic waste from 260,000 people and is licensed to receive industrial wastewater via sewer or tanker [11]. Example wastes that can be treated include high COD waste, landfill leachate, pharmaceutical and cosmetic wastes, chemical wastes, food wastes and other contaminated wastewater streams.

A screen shot from the E-PRTR query for the Blackburn sewage treatment works is provided in Figure S1. A summary of reported wastewater emissions to the River Darwen are presented in Table S1. These data if coupled with an estimate of river flow can be used to screen the potential risks posed by this point source discharge relative to other urban pollution sources.

Table S 1 Wastewater releases (kg/year) from 2010 to 2012 for the Blackburn sewage treatment works

Substance	**2012**	**2011**	**2010**
Arsenic	17.6	23.2	24.9
Chlorides	2540000	2340000	2260000
Copper	133	122	145
Diuron	1.91	2.01	2.03
Fluoride	7220	6640	6430
Nickel	129	95.2	88.7
Nonylphenol*	124	113	110
Lead	59.2	42.6	31.6
Pentachlorophenol	2.18	1.91	1.78
Zinc	759	596	531

*includes nonyl phenol ethoxylates

Facility details: UNITED UTILITIES WATER PLC, BLACKBURN STW

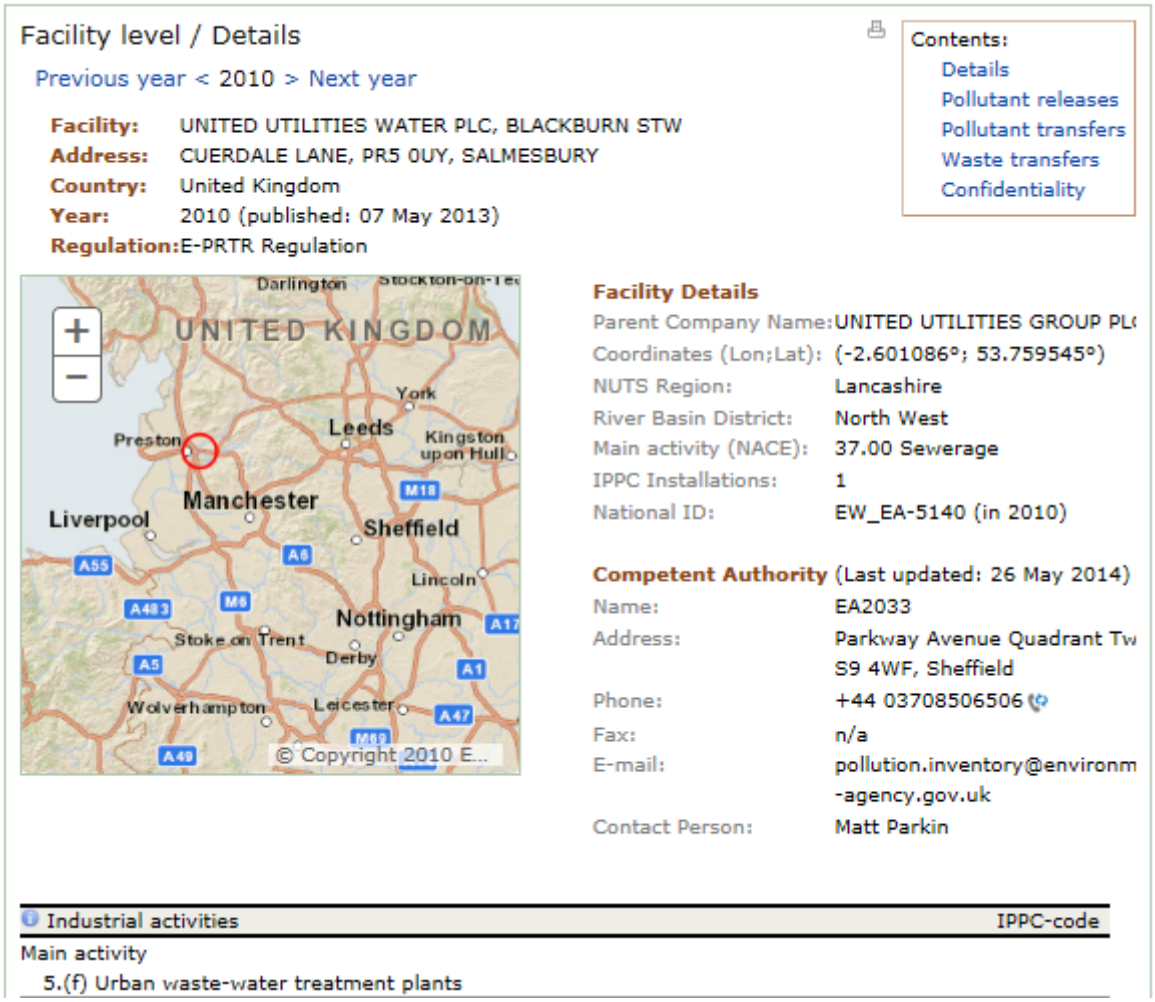

Figure S1. Results of E-PRTR search for the Blackburn sewage treatment works facility.

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