Supplementary Information for:

Prioritizing toxic shock threats to sewage treatment plants from down-the-drain industrial chemical spills: The RAVEN STREAM online tool

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Figure S1. Maps showing the approximate location of the study area of interest relative to northern Europe (insert) and map of the Käppala wastewater treatment plant service area in the Stockholm metropolitan area (primary map). Maps generated using Google Earth (insert) and EnvoMap® (Gemit Solutions).

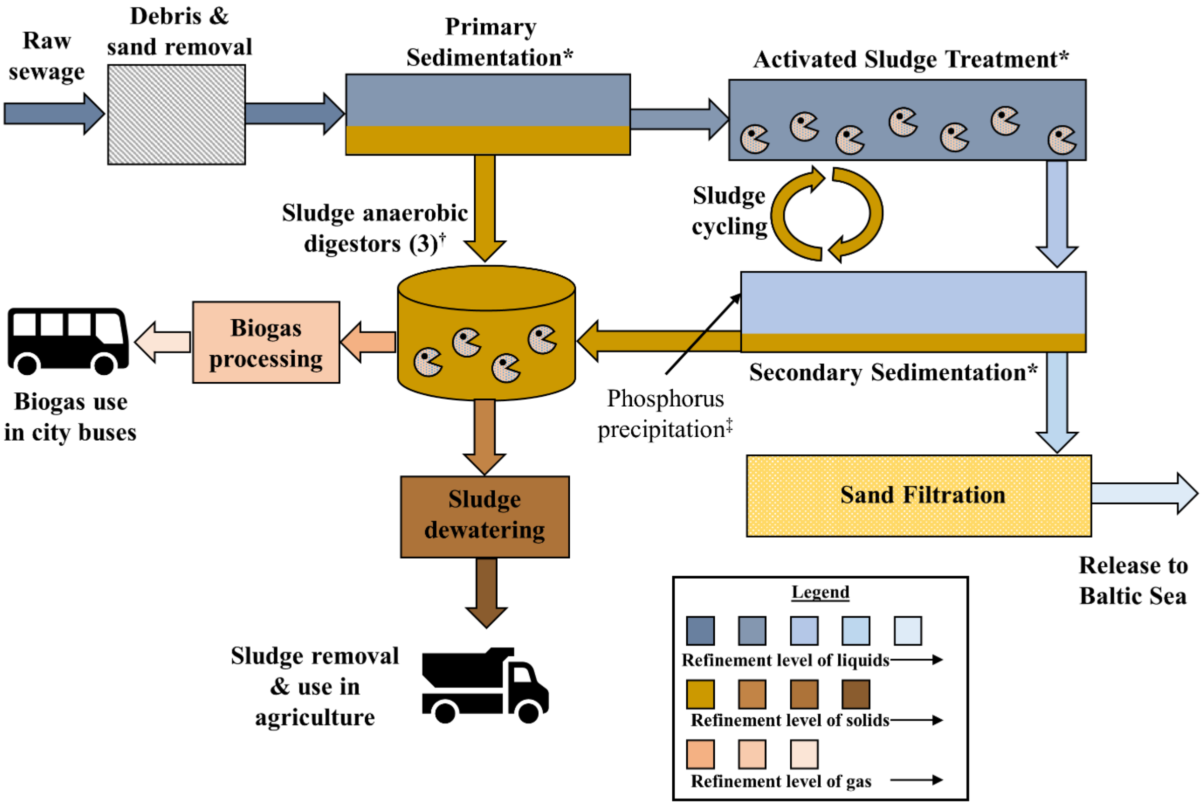

Figure S2. Schematic of the main elements of the Käppala sewage treatment plant processing steps. Microorganism-based treatment processes are employed in the activated sludge and anaerobic digestor regions. * There are 11 separate processing lines (6 in an older, smaller portion of the plant and 5 in a newer, larger region of the plant) within the primary sedimentation, activated sludge, and secondary sedimentation steps of the plant. † While there are 3 anaerobic digestors at the plant, at the time of the analysis only 2 were operational and so the volume reflecting these two was used for risk calculations. ‡ Chemical-induced phosphorus precipitation employs ferrous sulphate. Based on diagram in Käppala 2020[1].

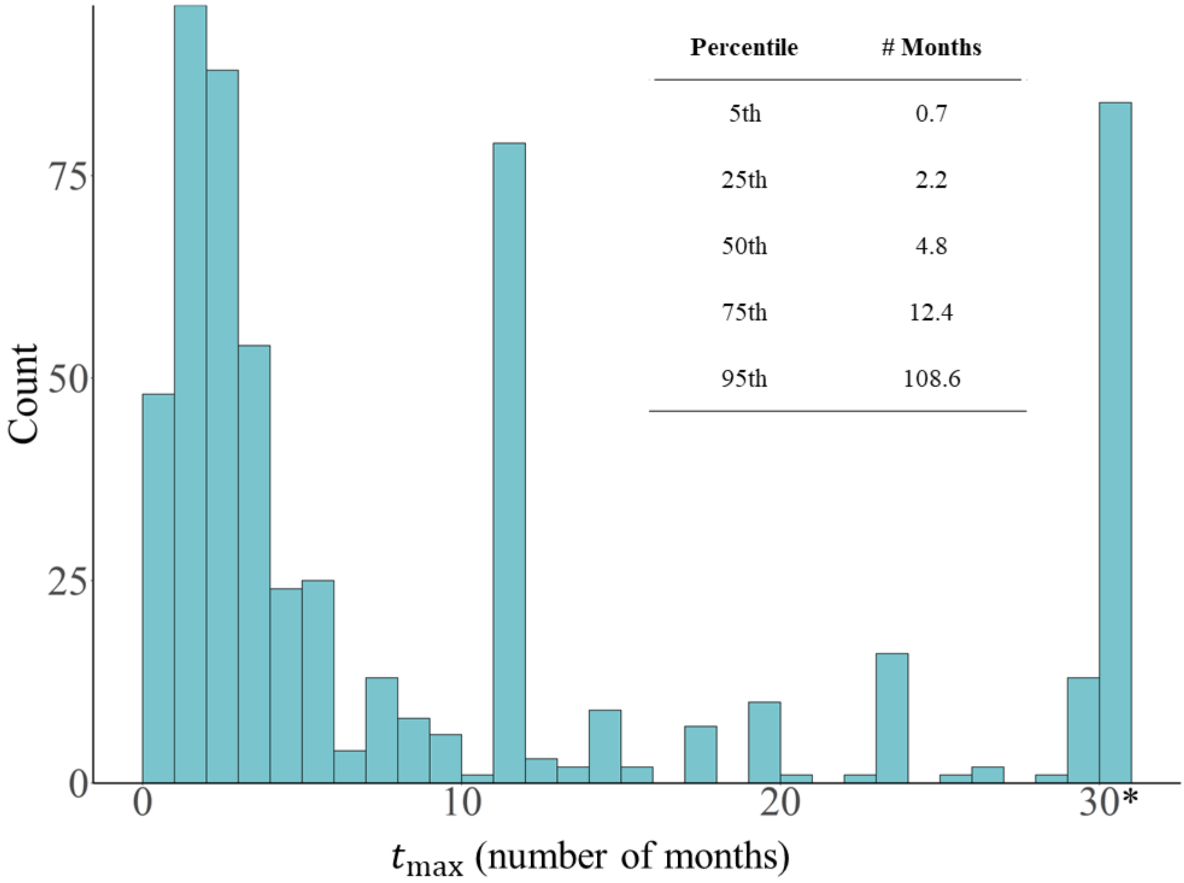

Figure S3. Distribution of the maximum number of months of industrial chemical product held in stock for the 598 products that have both max-in-stock and yearly usage data provided from the upstream industrial facility chemical use inventory conducted by Käppala. The inset table denotes a number of percentiles of the raw values of the plotted distribution (i.e., $t_{max}(x)$ calculated at various percentiles, see Section 2.1 of the main text for details). Figure generated using the R programming language package 'ggplot2'[2]. *All values above 30 months have been artificially compiled into the highest bin to enable easier visualization.

In situ measurements of a simulated chemical spill

A series of three tracer test experiments were carried out along the length of the Käppala Association's sewer network and surrounding area, with the locations of the three injection points shown in Figure S4. The first injection point (Experiment 1) was 9.1km upstream from the inlet of the STP. The second injection point (Experiment 2) was located in Sollentuna municipality, approximately 21.7km from the sample point. 0.8km of this distance was made up of the municipal network, rather than the primary tunnel network. The final injection point (Experiment 3) was close to Arlanda airport, approximately 45.9km from the inlet. For each Experiment, samples of influent sewage were taken at the inlet to Käppala as defined in Table S1. Collected samples were transferred into 4ml cuvettes, with some space left at the top of the cuvette for the buffer solution. A buffer solution (Titrisol; pH = 9) was added to bring the sample to within the pH range of maximum fluorescence, as the measurement of uranine concentration is pH sensitive[3]. Random testing of the pH level was carried out on numerous cuvettes to ensure the pH was above pH = 7. Additional Titrisol was added in the case that the pH was below this level. The cuvette was wiped using a fine cloth in order to remove dust, sample droplets, or fingerprints, which could cause interference. Uranine concentrations in the influent sewage samples were determined using a Jasco FP-777 spectrophotometer (serial number 071261; limit of detection of 0.002 ppb, or 2.0×10^{-9} g/l of uranine in deionised water). An excitation and emission wavelength of 493nm and 515nm, respectively, was used to determine uranine concentrations (fluorescence measurement accuracy of +/-1.5 nm, which is then converted to parts-per-billion concentration via a calibration curve). Tracer losses due to transit through the tunnel system to the inlet of the STP were calculated based on the known tracer injection mass, the measured concentrations of the tracer at the inlet, and the inflow rate of sewage into the STP during tracer sampling. See Scullin, 2021[4] for complete details on the tracer experiments.

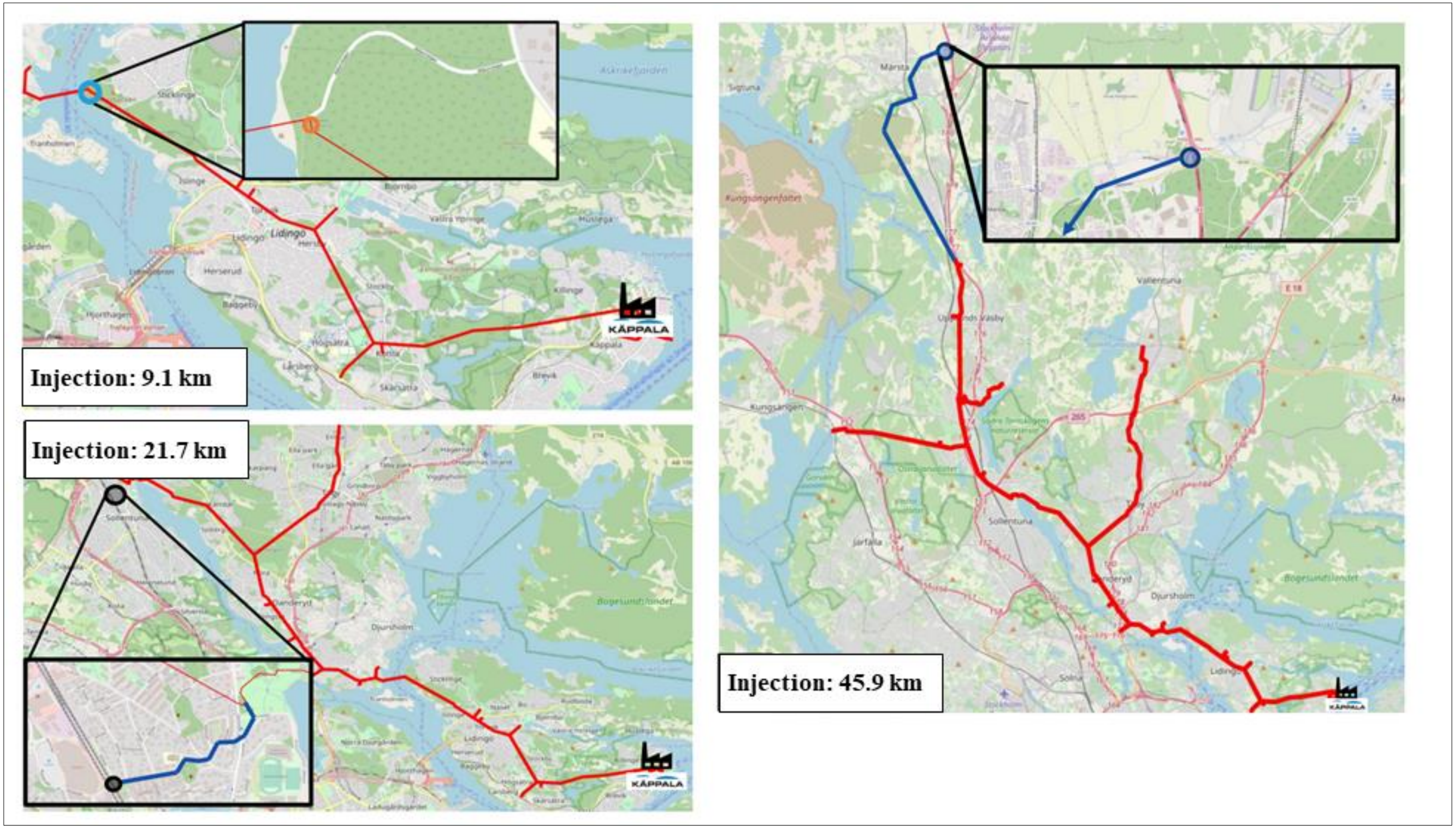

Figure S4. Locations of injection points for the uranine tracer chemical spill dilution experiments. Red lines show primary sewer tunnel (controlled by Käppala), while blue lines show the approximate location of relevant stretches of the municipal sewer network not under

Käppala’s control, but connected to the primary tunnel network. The injection at 9.1 km from Käppala is directly into the primary sewer tunnel, and the injection at 21.7 km is <1 km from the primary tunnel. For the injection at 45.9 km from Käppala, the municipal network connecting the injection point to the primary sewer tunnel exhibits similar characteristics to the primary sewer tunnel itself. Maps created using Envomap (Gemit Solutions). Adapted from Figure 9 of Scullin, 2021[4].

Table S1. Details associated with the uranine tracer chemical spill dilution experiments and inlet concentration sampling. All times are Stockholm local time.

Distance from injection to STP inlet (km)	Date	Time of injection	Sampling start time	Peak arrival time	Finish time	Minutes between samples	# of samples analysed*	Duration of injection (min)	Injection mass (kg)	Tracer losses (%)
9.1	2021-03-29	09:15	11:45	12:49	13:15	1	51	<1	1.045	25.7
21.7	2021-04-16	23:30	07:15	08:49	10:45	2	52	3	2.021	28.6
45.9	2021-04-28	11:00	07:17	07:53	10:45	4	50	2	4.002	33.2

* For each upstream chemical spill and inlet sampling experiment, the sampling rate was determined by modelling to predict the pattern of arrival of the tracer at the plant. Subsequently, 50-52 of the collected samples were visually analysed for levels of uranine and were deemed to most represent the breakthrough curve. This subset of the collected samples was sent for analysis. See Scullin, 2021[4] for full details.

Table S2. Risks posed to the three regions of the Käppala sewage treatment plant from constituent chemicals present in industrial chemical products used at the surveyed upstream industries, considering the high-end spill scenario. All chemicals that pose a risk value of 1 or more to the activated sludge regions are reported, however an additional 74 constituent chemicals pose a risk of over 1 to the anaerobic digestor region. The "Method" column indicates whether the max-in-stock industrial chemical product mass was reported by the industrial facility ("R") or estimated ("E") based on the method outlined in Section 2.1.2 of the main text. Risks are based on the use of the lowest sewage treatment plant predicted no effect concentration (i.e., highest toxicity) available for each chemical, and using the 50th percentile of $t_{max}(x)$ for instances where only yearly product usage was reported (see Sections 2.1 and 2.2 of the main text for details).

Facility Type & Product Number	Method	CAS Number	Smaller activated sludge region	Larger activated sludge region	Two anaerobic digestors
Energy plants 025	E	1305-78-8	2.5E+03	2.4E+03	1.9E+04
Energy plants 026	E	1305-62-0	1.2E+02	1.1E+02	9.1E+02
Disposal plants 060	E	1305-62-0	4.7E+01	4.4E+01	3.6E+02
Laundry 069	R	79-21-0	2.9E+01	2.7E+01	2.2E+02
Food industry 022	E	7487-88-9	1.6E+01	1.5E+01	1.2E+02
Energy plants 179	R	128-37-0	1.5E+01	1.4E+01	1.1E+02
Laundry 070	R	79-21-0	1.2E+01	1.1E+01	8.7E+01
Chem industries (1) 069	E	68439-46-3	1.1E+01	1.0E+01	8.2E+01
Energy plants 051	R	811-97-2	8.8E+00	8.2E+00	6.6E+01
Laundry 099	E	79-21-0	7.2E+00	6.7E+00	5.4E+01
Chem industries (2) 432	E	13463-41-7	6.8E+00	6.4E+00	5.1E+01

Chem industries (2) 174	E	9002-92-0	5.8E+00	5.5E+00	4.4E+01
Laundry 069	R	68609-93-8	4.2E+00	4.0E+00	3.2E+01
Chem industries (2) 300	E	64-17-5	3.0E+00	2.8E+00	2.3E+01
Chem industries (2) 500	E	124-68-5	2.3E+00	2.2E+00	1.7E+01
Food industry 023	E	7681-52-9	2.1E+00	1.9E+00	1.5E+01
Food industry 001	E	2372-82-9	2.0E+00	1.8E+00	1.5E+01
Energy plants 177	R	128-37-0	2.0E+00	1.8E+00	1.5E+01
Buses (3) 090	R	67762-38-3	1.8E+00	1.7E+00	1.4E+01
Chem industries (2) 522	E	541-02-6	1.8E+00	1.7E+00	1.4E+01
Chem industries (2) 007	E	115-10-6	1.6E+00	1.5E+00	1.2E+01
Chem industries (2) 392	E	77-54-3	1.3E+00	1.3E+00	1.0E+01
Food industry 009	E	7647-14-5	1.3E+00	1.3E+00	1.0E+01
Food industry 009	E	7647-14-5	1.3E+00	1.3E+00	1.0E+01
Chem industries (2) 081	E	112-02-7	1.2E+00	1.1E+00	9.1E+00
Laundry 069	R	7722-84-1	1.1E+00	1.0E+00	8.3E+00
Chem industries (2) 117	E	102-71-6	1.1E+00	1.0E+00	8.3E+00
Chem industries (1) 062	E	64-17-5	1.1E+00	1.0E+00	8.1E+00

Table S3. Risks posed to the three regions of the Käppala sewage treatment plant from industrial chemical products used at the surveyed upstream industries, assuming additive risks of the constituent chemicals and considering the same high-end spill scenario used for results shown in Table S2. All chemical products that pose a risk value of 1 or more to the activated sludge regions are reported, however an additional 72 chemical products pose a risk of at least 1 to the anaerobic digestor region. The "Method" column indicates whether the max-in-stock chemical mass was reported by the industrial facility ("R") or estimated ("E") based on the method outlined in Section 2.1.2 of the main text.

Facility Type & Product Number	Method	Smaller activated sludge region	Larger activated sludge region	Two anaerobic digestors
Energy plants 025	E	2.5E+03	2.4E+03	1.9E+04
Energy plants 026	E	1.2E+02	1.1E+02	9.1E+02
Disposal plants 060	E	4.7E+01	4.4E+01	3.6E+02
Laundry 069	R	3.4E+01	3.2E+01	2.6E+02
Food industry 022	E	1.6E+01	1.5E+01	1.2E+02
Energy plants 179	R	1.5E+01	1.4E+01	1.1E+02
Laundry 070	R	1.2E+01	1.1E+01	8.8E+01
Chem industries (1) 069	E	1.1E+01	1.0E+01	8.2E+01
Energy plants 051	R	8.8E+00	8.2E+00	6.6E+01
Laundry 099	E	7.4E+00	6.9E+00	5.5E+01
Chem industries (2) 432	E	6.8E+00	6.4E+00	5.1E+01
Chem industries (2) 174	E	5.8E+00	5.5E+00	4.4E+01
Chem industries (2) 300	E	3.1E+00	2.9E+00	2.3E+01
Food industry 009	E	2.7E+00	2.5E+00	2.0E+01

Chem industries (2) 500	E	2.3E+00	2.2E+00	1.7E+01
Food industry 023	E	2.1E+00	1.9E+00	1.5E+01
Food industry 001	E	2.0E+00	1.9E+00	1.5E+01
Energy plants 177	R	2.0E+00	1.8E+00	1.5E+01
Buses (3) 090	R	1.8E+00	1.7E+00	1.4E+01
Chem industries (2) 522	E	1.8E+00	1.7E+00	1.4E+01
Chem industries (2) 007	E	1.6E+00	1.5E+00	1.2E+01
Chem industries (2) 392	E	1.4E+00	1.3E+00	1.0E+01
Chem industries (2) 081	E	1.2E+00	1.1E+00	9.1E+00
Chem industries (2) 117	E	1.1E+00	1.0E+00	8.3E+00
Chem industries (1) 062	E	1.1E+00	1.0E+00	8.1E+00
Chem industries (2) 497	E	1.1E+00	9.8E-01	7.9E+00
Laundry 075	R	1.0E+00	9.6E-01	7.7E+00

References

1 Käppala, *The Käppala Association and the Käppala Wastewater Treatment Plant*, 2020. URL: https://www.kappala.se/globalassets/dokument/hjalp-oss-och-miljon/infomaterial/kappala_broschyr_english_tillg_webb.pdf

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