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Affinity of LDR Organics to Cementitious Materials: Sorption and Leaching Tests

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EXECUTIVE SUMMARY

SRNL is working to identify and test the physiochemical interactions of organic contaminants of potential concern with minerals in grout/cementitious materials. Organic species may interact with cementitious minerals including slag, fly ash, cement, and other components/dopants like carbon in fly ash. The identification of such interactions will support the solidification process design, performance assessments for the chemicals of concern, and a proposed Resource Conservation and Recovery Act (RCRA) treatment variance the technology-based treatment standard specified for the Land Disposal Restriction (LDR) organics associated with Hanford tank waste. In FY24, a list of the 132 reasonably expected to be present LDR organics associated with Hanford tank waste (RPP-RPT-63493, Rev 1a) was screened by functional groups, octanol-water partitioning coefficients, and detection frequency in Hanford tank waste samples. A subset of 10 compounds spanning the identified properties were tested using sorption and leachate tests. These compounds were subject to traditional batch sorption tests and leaching tests on/from Cast Stone cementitious material with and without activated carbon (a potential organic adsorption additive). The tests have been completed and analysis is underway but as yet currently unavailable. The analytical results (and conclusions) will be included in a forthcoming revision to this report as soon as they are available.

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LIST OF ABBREVIATIONS

HPLC	High Performance Liquid Chromatography
K_{ow}	Octanol-Water Partitioning Coefficient
LDR	Land Disposal Restricted
LAW	Low Activity Waste
PAHs	Polyaromatic Hydrocarbons
RCRA	Resource Conservation and Recovery Act
SRNL	Savannah River National Laboratory
SVOA	Semi-Volatile Organics Analysis
VOA	Volatile Organics Analysis
WRPS	Washington River Protection Solutions

1.0 Introduction

The Hanford site has approximately 54 to 56 million gallons of radioactive and hazardous waste stored in underground storage tanks. The Hanford Waste Treatment and Immobilization Plant is being built to treat the waste by separation into a low activity waste (LAW) and a high-level waste with subsequent vitrification of both components. While the baseline method for immobilization of LAW is vitrification, the current LAW vitrification facility is predicted to not have the capacity to immobilize all of the LAW. Alternate treatment of LAW by solidification/stabilization in a cementitious waste form is being investigated as a potential lower cost alternative to baseline vitrification. Application of an ambient temperature process rather vitrification creates the need to assess potential treatment options for Land Disposal Restricted (LDR) organic chemicals in Hanford LAW since thermal destruction by the vitrification process will no longer be part of the treatment train.[1]

Currently, the solidification/immobilization of organic molecules such as LDR organics is not a recognized treatment standard by the Environmental Protection Agency (40 CFR 268.42). However, in 2001, EPA provided notice of information concerning stabilization/immobilization of organics and a draft memorandum for comment.[†] The key paragraph in the draft memorandum is found in Section 2, paragraph (b) which states:

> *New adsorptive stabilization reagents such as modified clays, zeolites and specialized activated carbon have been specifically developed to entrap or immobilize certain types of hazardous organic constituents, particularly some of those found in contaminated soils. For the most part, the adsorbed organics cannot be easily desorbed. There are, however, certain conditions under which the adsorbed organics could desorb. For instance, co-disposal with other organic wastes could cause the adsorbed organics to desorb, and changes in the disposal conditions, such as fluctuations in pH, may have similar impacts. We recommend that stabilization reagents be examined on a site-specific basis to determine that they will be effective in the pH range expected in the leachate and that their adsorptive capacity would not be exceeded as the waste ages over time. These factors should be considered by the implementing regulatory agency. The use of these stabilization reagents to control the mobility of the hazardous organic constituents can thus be considered to provide substantial treatment through immobilization rather than being a type of impermissible dilution.*

While this memo was never finalized, it demonstrates that there has been historic recognition that there are physical and chemical interactions within cementitious matrices that can retain certain organic species. For this reason, Washington River Protection Solutions (WRPS) is working to develop a treatment variance specific for Hanford LAW to establish solidification/stabilization in cementitious waste forms that can provide acceptable treatment to that specified in 40 CFR 268.42 for some organic LDR constituents.

There are 132 LDR organics that are reasonably expected to be present in the Hanford LAW.[2] Establishing that some or all of these 132 LDR organics interact or are immobilized by cementitious materials through encapsulation, chemisorption, and other interactions (i.e. evaporation during setting) would support such a variance. However, previous studies of organic stabilization using cementitious materials (Portland cement, fly ash, slag) are largely waste/process specific, giving rise to mixed efficacy in treatment.[3-7] Therefore, process and compound (or groups of compounds) specific testing is requiring to support any proposed variance. The objectives of this study were fourfold:

[†] See 66 F.R. 52918 (October 18, 2001), and the Draft Interpretative Memorandum on the Stabilization of Organic-Bearing Hazardous Wastes dated September 2001 identified in the Federal Register notice. Although EPA requested comments on the draft memorandum, there is no record of EPA publishing the comments received or finalizing the memorandum so that the draft memorandum is the basis for this treatment variance petition demonstration.

1) Identify the possible interaction mechanisms that the 132 compounds could have with cementitious materials.
2) Group the compounds based on likely similarities in their interaction with cementitious materials.
3) Prioritize the 132 LDR organics associated with Hanford tank waste to help prioritize laboratory testing.
4) Test a select group of representative compounds for interactions with cementitious materials as a proof-of-concept.

Both sorption and leaching tests were used in this study to help isolate sorption and encapsulation effects during solidification/immobilization. Initial screening work grouping the 132 LDR organic species based on possible interaction mechanism with cementitious materials using the octanol water coefficient (K_{OW}) and compound structure. LDR organics associated with Hanford tank waste were grouped into five categories to help prioritize laboratory testing by detection frequency. Interactions of a subset of the compounds to Cast Stone cementitious materials were tested. The tests have been completed and analysis is underway but as yet currently unavailable. The analytical results (and conclusions) will be included in a forthcoming revision to this report as soon as they are available.

2.0 Quality Assurance

Requirements for performing reviews of technical reports and the extent of review are established in Savannah River Site manual E7 2.60. Savannah River National Laboratory (SRNL) documents the extent and type of review using the SRNL Technical Report Design Checklist contained in WSRC-IM-2002-00011, Rev. 2.

The work described in this report was requested by Washington River Protection Solutions (WRPS) in a Statement of Work (SOW).[8] An SRNL proposal was written in response of the SOWs.[9] This report documents Task 2 in the Task Technical and Quality Assurance Plan (TTQAP), Rev. 0 SRNL-RP-2024-00043.[10] Results are recorded in Electronic Laboratory Notebook L6390-00413-34.

3.0 Interaction Mechanisms

During immobilization/stabilization, cementitious material treats organic and inorganic species through both encapsulation and chemisorption. Encapsulation effects are the physical isolation of species wherein organic compounds may be held in the solid matrix, slowing their diffusion and advection of the waste form. Chemisorption is the chemical interaction of the organic species with the surface of the solids and is the result of chemical bonding between species and solid matrix. For chemisorption, organic compounds interact with solids though both absorption (into the solids) and adsorption (onto the solids). Cementitious materials have a variety of pore structures, so it is difficult to differentiate between absorption and adsorption. These will be referred to as “sorption” to encompass both processes.

Sorption of organics to cementitious materials during both the set/curing process and any potential gradual remobilization is defined by three underlying mechanisms: 1) ionic interactions with charged or partially charged sites on the surface[11], 2) hydrophobic forces driving the molecule out of the aqueous phase, and 3) van der Waals interactions between polar areas on the compound and solid surfaces.[12] For charged interactions, the high pH of both the LAW and the cementitious porewater/leachate (>13) results in either neutral or negatively charged organic molecules for all functional groups (e.g., carboxyl and hydroxyl) and net negative charge on the material surface. As such, minimal charge interactions are expected directly between the compound and the surface of the cementitious material (i.e. the pore water/cement interface). However, calcium has been shown to serve as a cation bridge between a negative charge site on compounds and those on the surface. This cation bridge facilitates sorption of negatively charged organic compounds and like-charged surface sites. Indeed, the negatively charged isosaccharinic acid has been shown to interact with calcium rich cementitious materials.[13] Van der Waals interactions are weak interactions between the polar compounds with polar portions of the surfaces. The compounds can be polar due to the presence of electron withdrawing or donating groups. These groups alter the electrostatic potential of the compound which may result in interaction of the compounds with heterogenous cement surfaces. This electrostatic potential alteration is most prominent for compounds containing benzene rings, resulting in stronger van der Waals interactions.[14] Finally, large organic molecules, such as Polyaromatic Hydrocarbons (PAHs), break up the hydrogen bonding structure of the bulk water phase. The hydration free energy to create this cavity or pocket within the hydrogen bonded water then drives the compounds out of the aqueous phase into other phases (e.g. solids). This entropic energy driven partitioning is often captured through octanol-water partitioning coefficients (K_{ow}) for compounds where high coefficients represent a high affinity for a hydrophobic environment. The K_{ow} for a compound can then be used as a qualitative proxy for the driving force out of solution. Whether the high electrolyte present in LAW and grout/cementitious material pore water decreases this energy by interrupting the bulk phase hydrogen bonding is unknown. Alternatively, the high electrolyte concentrations could increase the driving force from solution through processes akin to salting out effects seen for solubilities.

From these interaction mechanisms, the following compound characteristics were identified that may promote sorption of organic compounds to cementitious materials:

1) Presence of ionic groups at pH 13 or greater.
2) Presence of strong electron donating or withdrawing groups, especially attached to a benzene ring.
3) Large ring structures or high K_{ow} coefficients.

4.0 Interaction Mechanism Compound Grouping

4.1 Grouping Methods

The list of 132 LDR organics were screened for possible interactions with cementitious materials after collecting and reviewing K_{ow} (From Estimation programs interface suite [EPISuite][15]) and compound structures/functional groups. This screening focused on cementitious materials/minerals produced from cement, fly ash, and slag. For added organic material serving as a getter for the compounds as activated carbon was included below, the interactions are well understood.[12] Each compound was then assigned a numerical group signifying the possibility of interactions with cementitious materials where:

0 – Little to no interaction expected: These compounds are small polar molecules with low K_{ow} that would only be expected to interact through weak van der Waals interactions with the surface.
1 – Some interaction possible. Key characteristics for these compounds are the presence of benzene rings with polar functional groups enabling stronger van der Waals interactions, and K_{ow} in the middle of the range observed for the compounds studied.
2 – Interaction likely/expected. Key characteristics for these compounds are benzene rings and ionic (negatively charged) functional groups at the high pH, possibly facilitating a cation bridge with calcium to the surface.
3 – Large PAHs that would have a large driving force from the solution increasing retention and sorption on the solid phase.

4.2 Grouping Results

The results of the screening are provided in Appendix A. In summary, the screening identified:

- 40 group “0” compounds which are not expected to interact strongly with cementitious materials. These compounds may still be influenced by encapsulation effects.
- 37 group “1” compounds with some interaction possible.

- 39 group "2" compounds which were concluded to likely have interactions with the cementitious materials.
- 16 group "3" compound or those with high K_{ow} and multiple, conjoined aromatic rings creating large driving force out of solution.

5.0 Compound Prioritization

The list of 132 reasonably expected to be present LDR organics associated with Hanford tank waste were grouped into five categories to help prioritize laboratory testing. Category 1 represents the highest priority compounds for testing while Category 5 represents the lowest priority compounds. Table 5-1 provides a description of how compounds were grouped into each category. A list of the 132 reasonably expected to be present LDR organic compounds along with their corresponding categories is provided in Appendix B.

Table 5-1. Description of the Five Prioritization Categories

Category	Description	Number of Compound in Category
1	Compounds that have been detected in 5% or more of the Hanford tank waste sample in which they were included in the analyte list	18
2	Compounds that have been detected in between 1% and 5% of the Hanford tank waste samples in which they were included in the analyte list	19
3	Compounds not in Categories 1 or 2 but have been detected at least once and are soluble above their corresponding non-wastewater standard	16
4	Compounds not in Categories 1, 2, or 3 but are soluble above their corresponding non-wastewater standard and did not remain on the list of 132 solely because they either were included in the 1999 Data Quality Objective for the Tank Waste Remediation System Project (Rule 5 From RPP-RPT-63493) or were identified on and LDR notification form from past transfers into the double-shelled tank system (Rule 7 From RPP-RPT-63493)	28
5	Compounds not in Categories 1, 2, 3, or 4	51

6.0 Experimental Testing

6.1 Compound Selection

Compounds for sorption testing were selected to provide a broad range of possible interactions. Compounds were selected from each of the screening groups prioritizing compounds in high prioritization categories. Overall, 10 compounds were selected (Table 6-1) as part of an initial screening/proof-of-concept for these interactions. The screening results, detection grouping, and detection method to be used in this study are included for each compound. Note that 1,2-benzendicarboxylic acid (CAS# 88-99-3) was used for phthalic acid while 1,4-benzendicarboxylic acid is the isomer of concern.

Table 6-1. Compounds selected for proof-of-concept sorption testing

Name	CAS Number	pKa[A]	Log K_{ow}[B]	Charge (+,-,n) at pH 14	Functional Groups	Interaction Grouping (0, 1, 2, 3)	Prioritization Category	Detection Method
Phthalic acid (1,4-benzendicarboxylic acid)[C]	100-21-0	2.89, 5.51	2.00	2-	-COOH (x2)	2	4	HPLC
N-Nitrosomorpholine	59-89-2	stable	-0.44	n	-NN=O	0	1	VOA
2-Butanone	78-93-3	20	0.29	n	Ketone	0	1	VOA
1,2-Dichlorobenzene	95-50-1	>14	3.43	n	-Cl (x2),	1	3	VOA
2,4,6-Trichlorophenol	88-06-2	7	3.69	-	-Cl (x3), -OH	2	3	HPLC
4-Chloroaniline	106-47-8	3.98	1.83	n	-Cl, Amine	1	5	HPLC
Naphthalene	91-20-3	>30	3.3	n	ring structure	3	3	SVOA
Pentachlorophenol	87-86-5	5	5.12	-	-Cl (x5), -OH	2	2	HPLC
Toluene	108-88-3	>30	2.73	n		1	1	VOA
o-Cresol	95-48-7	10	1.95	-	-OH	1	4	HPLC

HPLC – High-performance liquid chromatography
VOA – Volatile Organic Analysis
SVOA - Semi Volatile Organic Analysis

A – From reference 16
B – From reference 15
C – Phallic acid (1,2-benzendicarboxylic acid, CAS# 88-99-3) was used for preliminary testing (K_{ow} = 0.73)

6.2 Methods

6.2.1 Cast Stone Preparation (Clean- and Organic-Containing)

Cast Stone was selected as the representative cementitious material. Cast Stone was made with 8% Type IL Portland cement from Lafarge, 47% blast furnace slag (Lafarge NUCEM Slag), and 45% fly ash from Centralia. Activated carbon as an additive to the Cast Stone formulation was also investigated by adding 1 weight percent (wt.(w%) activated carbon (Thermoscientific, -20+40 mesh).

The surrogate salt solution (waste simulant) selected was a 4M Na solution from PNNL-26165[17]. Oxalate was not included in the simulant for this series of tests to isolate any effect the organic anion may have on the sorption of the compound interactions. Once sorption affinities have been establish, testing with oxalate present will be performed in future testing. The component masses used to create the simulant are provided in Table 6-2. The simulant was prepared in 2 L batches and followed the chemical addition order used in SRNL-STI-2013-00541[18] and specified in Table 6-2. Each component was added and fully dissolved prior to adding the next component.

Table 6-2. 4M Na Salt Simulant Components

Order #	Compound	Amount (g / L)	Amount per 2 L batch (g)
1	Water	833.39	1666.78
2	$Al(NO_3)_3·9H_2O$	44.48	88.96
3	50% by Weight NaOH	118.51	237.02
4	Na_2SO_4	6.71	13.42
5	$Na_3PO_4·12H_2O$	11.73	23.46
7	Na_2CO_3	35.36	70.72
8	$NaNO_3$	77.83	155.66
9	$NaNO_2$	50.27	100.54
10	KCl	6.5	13

Both “clean” Cast Stone and organic-containing Cast Stone were made. For clean materials, 43.9 g of cement, 257.9 g of slag and 246.9 g of fly ash were added to a plastic bag and blended by hand until homogeneous. For activated carbon containing samples, 5.5 g (~1 wt%)of activated carbon was also added and blended. A water to premix ratio of 0.6 (w/w) was targeted by adding 424.6 g of salt simulant to a vessel. The blended dry materials were slowly added to the vessel while stirred by a Caframo overhead mixer with impeller attachment. Once visually homogenous, the slurry was poured into three 2” by 4” cylindrical molds and allowed to set. Importantly, the activated carbon did not float in the slurry and was well distributed into the monolithic form (Figure 6-1).

Organic-containing Cast Stone was formed by adding 100 mg organic compound per kg water (32.9 mg) to the simulant and allowing it to dissolve prior to adding the dry mix powders at a ratio of 0.6. Each compound was tested individually, which isolated specific compounds interactions. Mixtures of compound will need to be tested in the future. The target of 100 mg/kg water was used rather than 100 ppm (or 100 mg/L) to reduce the possibility of the organic salting out of solution. For naphthalene and 1,2-dichlorobenzene-dichlorobenzne which have solubilities below 100 ppm, 10 mg/kg water was targeted. A sample was also created with 100 mg naphthalene/kg water. For this sample, the naphthalene did not fully dissolve (as expected), and the dry powder was added with a small amount of discrete organic phases present.

Figure 6-1. Monoliths for Cast Stone (left) and activated carbon contained Cast Stone (right)

The samples were allowed to set and cure for 2 weeks. After 2 weeks, some samples still had bleed water present. This bleed water likely arose from the decreased free hydroxide content (< 0.4M) in the 4M Na simulant. In future testing, it is recommended that the water to dry blend ratio be decreased. The average amount of bleed water per batch (total of the 3 molds) was 3.5 g. Slightly more bleed water was seen for samples without activated carbon (5.9 g) compared to those containing activated carbon (1 g). The bleed water was collected after two-weeks of curing and submitted for analysis of organic constituents per methods in Table 6-1.

6.2.2 Sorption Tests

Sorption tests were performed for organic compounds onto the clean Cast Stone materials. After curing for 2 weeks, the monoliths were removed from the molds and size reduced/crushed. The crushed material was size-selected between 1.2 mm (16 mesh) and 9.5 mm (3/8 in). This size range was selected to remove fines (< 16 mesh) from the standard <3.8 in used for Toxic Characteristic Leaching Procedure.[19] The size selected material (20 g) was added to a 50 mL centrifuge tube. The individual stock solutions containing 100 ppm of each organic was prepared in volumetric flasks with DI water. For naphthalene and 1,2-dichlorobenzne, which have solubilities below 100 ppm, the stock solutions were 10 ppm. The stock solutions were spiked (20 mL) into the centrifuge tubes and placed on a shaker table at ambient temperature for 7 days. The tubes were then centrifuged and sampled. Once taken, samples were refrigerated before analysis to minimize losses of volatile compounds. The pH of each tube was also measured.

6.2.3 Leaching Tests

Crushed Cast Stone leachate tests were performed for the organic-containing Cast Stone materials. The crushed leachate tests were similar to the sorption tests in that the monoliths were removed after curing for 2 weeks and size reduced/crushed. The crushed material was size-selected between 1.2 mm and 9.5 mm. This size range was selected to remove fines (< 16 mesh) from the standard <3.8 in used for Toxic Characteristic Leaching Procedure.[19] Removing the fines aimed to remove isolate encapsulation effects (opposed to desorption from fines). The crushed material (20 g) was placed in centrifuge tubes and spiked with 20 mL of deionized water. The tubes were placed on a shaker table at ambient temperature for 7 days. The tubes were then centrifuged and sampled. Samples were refrigerated before analysis. The pH of each tube was also measured.

Monolith leach tests were also performed for the organic-containing cast stone forms. The monoliths were subjected to a modified United States EPA Manual SW-846 Method 1315 leach test.[20] The monoliths were suspended in 2-quart leachate buckets with deionized water for 7 days. Samples of the leachate were taken and analyzed. Samples were refrigerated before analysis.

6.3 Interim Results

The average pH for both the crushed sorption tests and leachate tests was 12.8 ± 0.1. No difference was seen in pH for samples containing the organic constituents or activated carbon. Unfortunately, at the time of this writing, results were not available from the organic analysis. Preliminary results show that some of the volatile compounds may have escaped the sorption and leachate systems. These results are being confirmed and troubleshooting is ongoing. The report will be revised when results are available.

7.0 Conclusions

Organic compounds are expected to interact with cementitious solids through, ionic, van der Waals and hydrophobic interactions. Screening results suggest that some of the LDR compounds reasonably expected to be present in Hanford LAW are likely to interact with cementitious solids. These interactions may constitute treatment in support of a variance. Analysis of sorption and leaching tests is underway.

8.0 Path Forward

Samples analysis will be completed shortly, and this report will be revised. Following this analysis, the proof-of-concept testing results will be used to identify any changes to the experimental methods needed for follow-on testing. Testing will also be extending to further compounds to establish trends and underlying mechanisms in physiochemical interactions between the organics of concern and cementitious materials. This will establish the ability of the LDR organics to be treated by solidification within a cementitious matrix in support or the proposed treatment variance to 40CFR 268.42.

In addition, future testing will include measuring retention factors (RF) for organics in the final solidified/stabilized waste forms by 1) testing for total concentration of an individual organic ($C_{i,total}$ in mg/kg) by exposing a representative sample of the waste form to an aggressive extractant, normally some type of solvent (e.g., SW-846 Methods 3540 Soxhlet Extraction[21] or 3541 Automated Soxhlet Extraction[22] for semi-volatile organics) and 2) by measuring the mass of the organic per unit sample mass that is released ($C_{i,released}$ in mg/kg) during EPA Method 1311 leach testing[19]. The retention factor is then given by:

$$RF_i = 1 - \frac{C_{i,released} \cdot M_{sample,TCLP}}{C_{i,total} \cdot M_{sample,total}}$$

Where $M_{sample,TCLP}$ is the mass of solid sample used EPA Method 1311 testing and $M_{sample,total}$ is the mass of solid sample used in measuring $C_{i,total}$.

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Appendix A. Organics Screening Results for the 132 Reasonably Expected to be Present LDR Organics

Name	CAS Number	Water Solubility (mg/L)^{A}	pKa^{A}	LogK$_{ow}$^{B}	K$_{ow}$ Source^{B}	Charge (+,-,n) at pH 14	Functional Groups	Interaction Grouping (0, 1, 2, 3)	Priority for Detection
Phthalic acid (1,4-benzendicarboxylic acid)	100-21-0	65	2.89, 5.51	0.73	Hansch,C et al. (1995)	2-	-COOH (x2)	2	4
2,4,5-Trichlorophenoxyacetic acid/2,4,5-TP	93-76-5	280	2.88 PubChem	3.31	KOWWIN v1.67 estimate	-	-COOH	2	5
N-Nitrosomorpholine	59-89-2	861527.5	stable	-0.44	Hansch,C et al. (1995)	n	-NN=O	0	1
N-Nitrosopyrrolidine	930-55-2	1000000	-3.14 Pred	-0.19	Hansch,C et al. (1995)	n	-NN=O	0	4
2-Naphthylamine	91-59-8	189	4.16	2.28	KOWWIN v1.67 estimate	n	ring structure, amine	3	5
1,4-Dinitrobenzene	100-25-4	13200	>14	-0.57	KOWWIN v1.67 estimate	n	Nitro (x2)	1	5
Benzo(g,h,i)perylene	191-24-2	0.00026375	>30	6.7	KOWWIN v1.67 estimate	n	ringstructure	3	5
bis(2-Chloroethoxy)methane	111-91-1	7800	>16.9	1.3	KOWWIN v1.67 estimate	n	-Cl (x2), ether	1	5
2-sec-Butyl-4,6-dinitrophenol/Dinoseb	88-85-7	50	4.62	3.56	WSSA (1983)	n	-OH, Nitro (x2)	2	5
p-Cresidine	120-71-8	2810	4.66 Pred	1.74	Hansch,C et al. (1995)	n	amine	1	5

Name	CAS Number	Water Solubility (mg/L)[A]	pKa[A]	LogK$_{ow}$[B]	K$_{ow}$ Source[B]	Charge (+,-,n) at pH 14	Functional Groups	Interaction Grouping (0, 1, 2, 3)	Priority for Detection
N-Nitrosopiperidine	100-75-4	76480	(-3.2 Pred)	0.36	Hansch,C et al. (1995)	n	-NN=O	0	4
N-Nitrosodimethylamine	62-75-9	1000000	>30	-0.57	Hansch,C et al. (1995)	n	-NN=O	0	1
4,6-Dinitro-o-cresol	534-52-1	130	5	2.13	Hansch,C et al. (1995)	-	-OH, Nitro (x2)	1	3
Cresols (m,p,o)	1319-77-3	31800	10	1.94	Hansch,C et al. (1995)	-	-OH	1	4
N-Nitrosomethylethylamine	10595-95-6	300000	<1, >30	0.04	Vera,A et al. (1992)	n	-NN=O	0	4
2,4-Dimethylaniline (2,4-xylidine)	95-68-1	6150	4.89	1.68	Hansch,C et al. (1995)	n	amine (1st)	1	5
Diphenylamine	122-39-4	55	0.78	3.5	Hansch,C et al. (1995)	n	anime (2nd)	2	2
gamma-BHC	58-89-9	7.8	>30	3.72	Hansch,C et al. (1995)	n	-Cl (x6)	2	5
N-Nitrosodiethylamine	55-18-5	106000	<1, >30	0.48	Hansch,C et al. (1995)	n	-NN=O	0	4
Endrin aldehyde	7421-93-4	0.024	>14	5.73	KOWWIN v1.67 estimate	n	Ketone, -Cl (X6)	2	5

Name	**CAS Number**	**Water Solubility (mg/L)**[A]	**pKa**[A]	**LogK$_{ow}$**[B]	**K$_{ow}$ Source**[B]	**Charge (+,-,n) at pH 14**	**Functional Groups**	**Interaction Grouping (0, 1, 2, 3)**	**Priority for Detection**
Methanol	67-56-1	Miscible	16	-0.77	Hansch,C et al. (1995)	n	-OH	0	4
1,4-Dioxane	123-91-1	Miscible	>14	-0.27	Hansch,C et al. (1995)	n	cyclic ether	0	5
beta-BHC	319-85-7	0.2	>30	3.72	Hansch,C et al. (1995)	n	-Cl (x6)	2	5
delta-BHC	319-86-8	10.7	>30	3.72	Hansch,C et al. (1995)	n	-Cl (x6)	2	5
3-Methylcholanthrene	56-49-5	0.002586537	>30	6.42	Hansch,C et al. (1995)	n	ringstructure	3	5
p,p′-DDD	72-54-8	0.062823355	>14	6.02	Sangster (1994)	n	-Cl (x4)	2	5
n-Butyl alcohol	71-36-3	79000	16	0.88	Hansch,C et al. (1995)	n	-OH	0	1
alpha-BHC	319-84-6	1.8	>30	4.14	Hansch,C et al. (1995)	n	-Cl (x6)	2	5
Pyridine	110-86-1	455172.9904	5.25	0.65	Hansch,C et al. (1995)	n	heterocyclic amine	1	2

Name	**CAS Number**	**Water Solubility (mg/L)[A]**	**pKa[A]**	**LogK$_{ow}$[B]**	**K$_{ow}$ Source[B]**	**Charge (+,-,n) at pH 14**	**Functional Groups**	**Interaction Grouping (0, 1, 2, 3)**	**Priority for Detection**
Cyclohexanone	108-94-1	105000	16.7	0.81	Hansch,C et al. (1995)	n	ketone	0	1
Dieldrin	60-57-1	0.2324817	>14	5.4	DeBruijn,J et al. (1989)	n	-Cl (x6), Epoxide	2	5
Isobutyl alcohol	78-83-1	88000	16	0.77	Hansch,C et al. (1995)	n	-OH	1	4
Aldrin	309-00-2	0.138202899	>30	6.5	DeBruijn,J et al. (1989)	n	-Cl (x6)	2	5
Acetonitrile	75-05-8	Miscible	alkaline hydrolysis	-0.34	Hansch,C et al. (1995)	n	Nitriles	0	1
Heptachlor epoxide	1024-57-3	0.2	>30	NA	NA	n	-Cl (x7), epoxide	2	5
p,p′-DDT	50-29-3	0.010321607	>14	6.79	Hansch,C et al. (1995)	n	-Cl (x5)	2	5
Ethyl cyanide/Propanenitrile	107-12-0	115000	alkaline hydrolysis	0.35	Hansch,C et al. (1995)	n	Nitriles	0	4
p,p′-DDE	72-55-9	0.054759086	>14	6	Sangster (1993)	n	-Cl (x4)	2	5
Isodrin	465-73-6	0.014	>14	6.75	DeBruijn,J et al. (1989)	n	-Cl (x6)	2	5

Name	CAS Number	Water Solubility (mg/L)^A	pKa^A	LogK$_{ow}$^{B}	K$_{ow}$ Source^B	Charge (+,-,n) at pH 14	Functional Groups	Interaction Grouping (0, 1, 2, 3)	Priority for Detection
Acenaphthylene	208-96-8	14.09893389	>30	3.94	Hansch,C et al. (1995)	n	ringstructure	2	5
Acrolein	107-02-8	263000	>30	-0.01	Hansch,C et al. (1995)	n	Aldehyde	0	5
Ethyl acetate	141-78-6	87900	alkaline hydrolysis	0.73	Hansch,C et al. (1995)	n	Ester	0	4
Methacrylonitrile	126-98-7	26400	alkaline hydrolysis	0.68	Tanii,H & Hashimoto,K (1984)	n	cynidide	0	4
1,2-Dibromoethane/Ethylene dibromide	106-93-4	4140	alkaline hydrolysis	1.96	Hansch,C et al. (1995)	n	-Br (X2)	0	4
Ethyl Ether	60-29-7	63000	>30	0.89	Hansch,C et al. (1995)	n	ether	0	4
1,1,1,2-Tetrachloroethane	630-20-6	1070	>14	2.93	KOWWIN v1.67 estimate	n	-Cl (x4)	1	5
trans-1,3-Dichloropropylene	10061-02-6	2800	alkaline hydrolysis	2.06	Tomlin,C (1997)	n	-Cl (x2)	0	3
Xylene(m,p,o)	1330-20-7	175	>30	3.2	Hansch,C et al. (1995)	n		1	1
2-Chloroethyl vinyl ether	110-75-8	429	>14	1.17	KOWWIN v1.67 estimate	n	Ether, -Cl	0	5
3-Chloropropylene	107-05-1	4000	alkaline hydrolysis	1.93	KOWWIN v1.67 estimate	n	-Cl	0	4

Name	**CAS Number**	**Water Solubility (mg/L)**[A]	**pKa**[A]	**LogK_{ow}**[B]	**K_{ow} Source**[B]	**Charge (+,-,n) at pH 14**	**Functional Groups**	**Interaction Grouping (0, 1, 2, 3)**	**Priority for Detection**
1,1,2-Trichloro-1,2,2-trifluroethane	76-13-1	170	>14	3.16	Hansch,C et al. (1995)	n	-Cl (x3), -F (x3)	0	2
1,1,1-Trichloroethane	71-55-6	1290	>30	2.49	Hansch,C et al. (1995)	n	-Cl (x3)	0	1
1,1-Dichloroethylene	75-35-4	2420	>30	2.13	Hansch,C et al. (1995)	n	-Cl (x2)	0	3
1,2-Dichloroethane	107-06-2	8600	>30	1.48	Hansch,C et al. (1995)	n	-Cl (x2)	0	3
2,4,5-Trichlorophenol	95-95-4	1000	7	3.72	Hansch,C et al. (1995)	-	-Cl (x3), -OH	2	3
2,4-Dinitrotoluene	121-14-2	270	13.5	-0.02	KOWWIN v1.67 estimate	n	Nitro (X2)	1	4
2-Butanone	78-93-3	344000	20	0.29	Hansch,C et al. (1995)	n	Ketone	0	1
4-Methyl-2-pentanone	108-10-1	18800	20	1.31	Tanii,H & Hashimoto,K (1986)	n	Ketone	0	2
Acetone	67-64-1	Miscible	20	-0.24	Hansch,C et al. (1995)	n	Ketone	0	1
All Aroclors: Pentachlorobiphenyl	1336-36-3	0.7	>30	6.98	KOWWIN v1.67 estimate	n	-Cl (x5)	2	2

Name	**CAS Number**	**Water Solubility (mg/L)^A**	**pKa^A**	**LogK$_{ow}$^{B}**	**K$_{ow}$ Source^B**	**Charge (+,-,n) at pH 14**	**Functional Groups**	**Interaction Grouping (0, 1, 2, 3)**	**Priority for Detection**
Benzene	71-43-2	1770	>30	2.13	Hansch,C et al. (1995)	n		2	1
Butyl benzyl phalate	85-68-7	2.69	alkaline hydrolysis	4.73	Ellington,JJ & Floyd,TL (1996)	-	Ester(x2)	2	1
Carbon tetrachloride	56-23-5	650	>30	2.83	Hansch,C et al. (1995)	n	-Cl (x4)	1	3
Chloroform	67-66-3	8000	16	1.97	Hansch,C et al. (1995)	n	-Cl (x3)	1	3
di-n-Butyl phthalate	84-74-2	11.2	alkaline hydrolysis	4.5	Ellington,JJ & Floyd,TL (1996)	-	Ester(x2)	2	1
Hexachlorobutadiene	87-68-3	4100	>30	4.78	Hansch,C et al. (1995)	n	-Cl (x6)	1	4
Hexachloroethane	67-72-1	50	>30	4.14	Hansch,C et al. (1995)	n	-Cl (x6)	0	4
Methylene chloride	75-09-2	17600	>30	1.25	Hansch,C et al. (1995)	n	-Cl (x2)	0	1
Nitrobenzene	98-95-3	3395	>30	-0.39	KOWWIN v1.67 estimate	n	Nitro	1	3
Tetrachloroethylene	127-18-4	286	20 - 30	3.4	Hansch,C et al. (1995)	n	-Cl (x4)	0	3
Trichloroethylene	79-01-6	1280	20 - 30	2.42	Hansch,C et al. (1995)	n	-Cl (x3)	0	2

Name	CAS Number	Water Solubility (mg/L)^A	pKa^A	LogK$_{ow}$^{B}	K$_{ow}$ Source^B	Charge (+,-,n) at pH 14	Functional Groups	Interaction Grouping (0, 1, 2, 3)	Priority for Detection
Vinyl chloride	75-01-4	2700	>30	1.62	KOWWIN v1.67 estimate	n	-Cl	0	4
1,1,2,2-Tetrachloroethane	79-34-5	2830	20 - 30	2.18	Hansch,C et al. (1995)	n	-Cl (x4)	0	4
1,1,2-Trichloroethane	79-00-5	4590	20 - 30	1.89	Hansch,C et al. (1995)	n	-Cl (x3)	0	3
1,1-Dichloroethane	75-34-3	5000	>30	1.79	Hansch,C et al. (1995)	n	-Cl (x2)	0	4
1,2,4-Trichlorobenzene	120-82-1	37	>30	4.02	Hansch,C et al. (1995)	n	-Cl (x3)	1	1
1,2-Dichlorobenzene	95-50-1	150	>14	3.43	Hansch,C et al. (1995)	n	-Cl (x2)	1	3
1,3-Dichlorobenzene	541-73-1	103	>30	3.53	Hansch,C et al. (1995)	n	-Cl (x2)	1	2
1,4-Dichlorobenzene	106-46-7	80	>30	3.44	Hansch,C et al. (1995)	n	-Cl (x2)	1	2
2,4,6-Trichlorophenol	88-06-2	690	7	3.69	Hansch,C et al. (1995	-	-Cl (x3), -OH	2	3
2,4-Dichlorophenol	120-83-2	5500	7.89	3.06	Hansch,C et al. (1995)	-	-Cl (x2), -OH	2	5
2,4-Dimethyl phenol	105-67-9	7870	10.6	2.3	Hansch,C et al. (1995)	-	-OH	2	5
2,4-Dinitrophenol	51-28-5	69	5	1.67	Hansch,C et al. (1995)	-	Nitro (x2), -OH	2	1

Name	CAS Number	Water Solubility (mg/L)^A	pKa^A	LogK$_{ow}$^B	K$_{ow}$ Source^B	Charge (+,-,n) at pH 14	Functional Groups	Interaction Grouping (0, 1, 2, 3)	Priority for Detection
2-Chloronaphthalene	91-58-7	11.74002657	>14	4.14	Hansch,C et al. (1995)	n	-Cl, ringstructure	3	5
2-Chlorophenol	95-57-8	23200	8.56	2.15	Hansch,C et al. (1995)	-	-OH, -Cl	2	3
2-Nitroaniline	88-74-4	14900	(-0.28)	1.85	Hansch,C et al. (1995)	n	Nitro, Amide	1	3
2-Nitrophenol	88-75-5	1700	7	1.79	Hansch,C et al. (1995)	-	Nitro, -OH	1	2
4-Bromophenyl phenyl ether	101-55-3	Insoluble	>14	4.94	KOWWIN v1.67 estimate	n	Ether, -Br	2	5
4-Chloroaniline	106-47-8	2990	3.98	1.83	Hansch,C et al. (1995)	n	-Cl, Amide	1	5
4-Nitroaniline	100-01-6	730	12.99	1.39	Hansch,C et al. (1995)	n	Nitro, Amide	1	2
Acenaphthene	83-32-9	3.902446465	>30,	3.92	Hansch,C et al. (1995)	n	ringstructure	3	5
Anthracene	120-12-7	0.057508217	>30	4.45	Hansch,C et al. (1995)	n	ringstructure	3	5
Benz(a)anthracene	56-55-3	0.011266667	>30	5.76	Wang,L et al. (1986)	n	ringstructure	3	5
Benzo(a)pyrene	50-32-8	0.00293	>30	5.99	KOWWIN v1.67 estimate	n	ringstructure	3	5
Benzo(b)fluoranthene	205-99-2	0.002334286	>30	5.78	Wang,L et al. (1986)	n	ringstructure	3	5

Name	**CAS Number**	**Water Solubility (mg/L)^A**	**pKa^A**	**LogK$_{ow}$^{B}**	**K$_{ow}$ Source^B**	**Charge (+,-,n) at pH 14**	**Functional Groups**	**Interaction Grouping (0, 1, 2, 3)**	**Priority for Detection**
Benzo(k)fluoranthene	207-08-9	0.001885	>30	6.11	De Maagd PG et al. (1988) (not in chemspider)	n	ringstructure	3	5
bis(2-Chloroethyl)ether	111-44-4	10500	>30	1.29	Hansch,C et al. (1995) (not in chemspider)	n	Ether, -Cl	1	5
bis(2-ethylhexyl)phthalate	117-81-7	0.27	alkaline hydrolysis	9.52	KOWWIN v1.67 estimate	-	Ester (x2), Hydrocarbon chain	2	1
Chlorobenzene	108-90-7	500	>30	2.84	Sangster (1994)	n	-Cl	1	2
Chloroethane	75-00-3	6700	stable	1.43	Hansch,C et al. (1995)	n	-Cl	0	4
Chloromethane	74-87-3	5350	>30	0.91	Hansch,C et al. (1995)	n	-Cl	0	2
Chrysene	218-01-9	0.002953639	>30	5.81	De Maagd,PG et al. (1998)	n	ringstructure	3	5
cis-1,3-Dichloropropylene	10061-01-5	2700	alkaline hydrolysis	2.03	Tomlin,C (1997)	n	-Cl (x2)	1	4
Dibenzo(a,h)anthracene	53-70-3	0.0011	>30	6.54	Helweg,C et al. (1997a)	n	ringstructure	2	5
Diethyl phthalate	84-66-2	1200	alk hydrolysis	2.47	Hansch,C et al. (1995)	-	Ester (x2)	2	1
Dimethyl phthalate	131-11-3	3590	alk hydrolysis	1.6	Ellington,JJ & Floyd,TL (1996)	-	Ester (x2)	2	5

Name	CAS Number	Water Solubility (mg/L)[A]	pKa[A]	LogK$_{ow}$[B]	K$_{ow}$ Source[B]	Charge (+,-,n) at pH 14	Functional Groups	Interaction Grouping (0, 1, 2, 3)	Priority for Detection
Di-n-octyl phthalate	117-84-0	0.02	alk hydrolysis	8.1	Ellington,JJ & Floyd,TL (1996)	-	Ester (x2), Hydrocarbon chain	2	2
Ethyl benzene	100-41-4	161	>30	3.15	Hansch,C et al. (1995)	n		1	2
Fluoranthene	206-44-0	0.240715434	>30	5.16	Hansch,C et al. (1995)	n	ringstructure	2	5
Fluorene	86-73-7	1.897724094	>30, PAH	4.18	Hansch,C et al. (1995)	n	ringstructure	3	5
Hexachlorobenzene	118-74-1	0.0096	no hydrogens	5.73	DeBruijn,J et al. (1989)	n	-Cl (x2)	2	5
Hexachlorocyclopentadiene	77-47-4	1.8	no hydrogens	5.04	Hansch,C et al. (1995)	n	-Cl	2	5
Indeno(1,2,3-c,d) pyrene	193-39-5	0.017851429	>30	6.7	EPIsuite	n	ringstructure	3	5
Naphthalene	91-20-3	31.61534708	>30	3.3	Hansch,C et al. (1995)	n	ringstructure	3	3
N-Nitroso-di-n-propylamine	621-64-7	9890	stable	1.36	Hansch,C et al. (1995)	n	-NN=O	0	2
Pentachlorophenol	87-86-5	21	5	5.12	Hansch,C et al. (1995)	-	-Cl (x5), -OH	2	2
Phenanthrene	85-01-8	1.168957496	>30	4.46	Hansch,C et al. (1995)	n	ringstructure	3	5

Name	CAS Number	Water Solubility (mg/L)[A]	pKa[A]	LogK_{ow}[B]	K_{ow} Source[B]	Charge (+,-,n) at pH 14	Functional Groups	Interaction Grouping (0, 1, 2, 3)	Priority for Detection
Phenol	108-95-2	91700	10	1.46	Hansch,C et al. (1995)	-	-OH	1	2
p-Nitrophenol	100-02-7	15800	7.15	1.91	Hansch,C et al. (1995)	-	-OH, Nitro	1	2
Pyrene	129-00-0	0.136978602	>30, PAH	4.88	Hansch,C et al. (1995)	n	ringstructure	3	2
Toluene	108-88-3	519	>30	2.73	Hansch,C et al. (1995)	n		1	1
Trichlorofluoromethane	75-69-4	1100	>30	2.53	Hansch,C et al. (1995)	n	-F, -Cl (x3)	0	4
N-Nitroso-di-n-butylamine	924-16-3	1270	(-3.14)	2.63	Hansch,C et al. (1995)	n	-NN=O, hydrocarbon chain	1	4
Pentachloronitrobenzene	82-68-8	0.44	no hydrogens	4.64	Sangster (1994)	n	-Cl (x5), Nitro	1	5
1,2,4,5-Tetrachlorobenzene	95-94-3	0.6	>14, stable	4.6	Hansch,C et al. (1995)	n	-Cl (x4)	2	5
2,3,4,6-Tetrachlorophenol	58-90-2	170	5.22	4.45	Hansch,C et al. (1995)	-	-Cl (x4), -OH	2	5
Acetophenone	98-86-2	7780	16	1.58	Hansch,C et al. (1995)	n	Ketone	1	5
Acrylonitrile	107-13-1	79300	>14	0.25	Hansch,C et al. (1995)	-	Nitrile	0	4
p-Chloro-m-cresol	59-50-7	4000	9.55	3.1	Hansch,C et al. (1995)	-	-Cl, -OH	1	3

Name	**CAS Number**	**Water Solubility (mg/L)**[A]	**pKa**[A]	**LogK_{ow}**[B]	**K_{ow} Source**[B]	**Charge (+,-,n) at pH 14**	**Functional Groups**	**Interaction Grouping (0, 1, 2, 3)**	**Priority for Detection**
o-Cresol	95-48-7	31800	10	1.95	Hansch,C et al. (1995)	-	-OH	1	4
m-Cresol	108-39-4	25700	10	1.96	Hansch,C et al. (1995)	-	-OH	1	4
p-Cresol	106-44-5	23100	10	1.94	Hansch,C et al. (1995)	-	-OH	1	4

A- See reference [23] for details
B - From EPISuite[15]
NA = Not available

Appendix B: Compound Prioritization Category Determination

Name	CAS Number	Detection Frequency (%)	Category
Acetone	67-64-1	64.3%	1
Acetonitrile	75-05-8	41.7%	1
n-Butyl alcohol	71-36-3	38.7%	1
2-Butanone	78-93-3	38.1%	1
Toluene	108-88-3	30.1%	1
Methylene chloride	75-09-2	28.2%	1
Xylene(m,p,o)	1330-20-7	24.7%	1
N-Nitrosodimethylamine	62-75-9	20.2%	1
2,4-Dinitrophenol	51-28-5	10.9%	1
Benzene	71-43-2	10.6%	1
N-Nitrosomorpholine	59-89-2	9.8%	1
1,1,1-Trichloroethane	71-55-6	9.7%	1
Diethyl phthalate	84-66-2	6.5%	1
Cyclohexanone	108-94-1	6.4%	1
1,2,4-Trichlorobenzene	120-82-1	5.0%	1
4-Methyl-2-pentanone	108-10-1	3.7%	2
1,3-Dichlorobenzene	541-73-1	3.7%	2
Diphenylamine	122-39-4	3.5%	2
Pentachlorophenol	87-86-5	3.0%	2
Chlorobenzene	108-90-7	3.0%	2
Pyridine	110-86-1	2.7%	2
Trichloroethylene	79-01-6	1.7%	2
1,4-Dichlorobenzene	106-46-7	1.6%	2
Phenol	108-95-2	1.6%	2
Ethyl benzene	100-41-4	1.4%	2
2-Nitrophenol	88-75-5	1.3%	2
p-Nitrophenol	100-02-7	1.3%	2
N-Nitroso-di-n-propylamine	621-64-7	1.3%	2
1,1,2-Trichloro-1,2,2-trifluroethane	76-13-1	1.2%	2
Chloromethane	74-87-3	1.0%	2
4-Nitroaniline	100-01-6	1.0%	2
Chloroform	67-66-3	0.9%	3
1,2-Dichloroethane	107-06-2	0.9%	3
Naphthalene	91-20-3	0.9%	3
Nitrobenzene	98-95-3	0.8%	3
2-Nitroaniline	88-74-4	0.5%	3
4,6-Dinitro-o-cresol	534-52-1	0.5%	3
1,1,2-Trichloroethane	79-00-5	0.5%	3

Name	**CAS Number**	**Detection Frequency (%)**	**Category**
trans-1,3-Dichloropropylene	10061-02-6	0.5%	3
Tetrachloroethylene	127-18-4	0.4%	3
Carbon tetrachloride	56-23-5	0.4%	3
2,4,6-Trichlorophenol	88-06-2	0.4%	3
2-Chlorophenol	95-57-8	0.4%	3
2,4,5-Trichlorophenol	95-95-4	0.4%	3
p-Chloro-m-cresol	59-50-7	0.4%	3
1,1-Dichloroethylene	75-35-4	0.4%	3
1,2-Dichlorobenzene	95-50-1	0.4%	3
1,1,2,2-Tetrachloroethane	79-34-5	0.0%	4
1,1-Dichloroethane	75-34-3	0.0%	4
1,2-Dibromoethane/Ethylene dibromide	106-93-4	0.0%	4
2,4-Dinitrotoluene	121-14-2	0.0%	4
3-Chloropropylene	107-05-1	0.0%	4
Acrylonitrile	107-13-1	0.0%	4
Chloroethane	75-00-3	0.0%	4
cis-1,3-Dichloropropylene	10061-01-5	0.0%	4
Cresols (m,p,o)	1319-77-3	0.0%	4
Ethyl acetate	141-78-6	0.0%	4
Ethyl cyanide/Propanenitrile	107-12-0	0.0%	4
Ethyl Ether	60-29-7	0.0%	4
Hexachlorobutadiene	87-68-3	0.0%	4
Hexachloroethane	67-72-1	0.0%	4
Isobutyl alcohol	78-83-1	0.0%	4
m-Cresol	108-39-4	0.0%	4
Methacrylonitrile	126-98-7	0.0%	4
Methanol	67-56-1	0.0%	4
N-Nitrosodiethylamine	55-18-5	0.0%	4
N-Nitroso-di-n-butylamine	924-16-3	0.0%	4
N-Nitrosomethylethylamine	10595-95-6	0.0%	4
N-Nitrosopiperidine	100-75-4	0.0%	4
N-Nitrosopyrrolidine	930-55-2	0.0%	4
o-Cresol	95-48-7	0.0%	4
p-Cresol	106-44-5	0.0%	4
Phthalic acid	88-99-3	0.0%	4
Trichlorofluoromethane	75-69-4	0.0%	4
Vinyl chloride	75-01-4	0.0%	4
1,1,1,2-Tetrachloroethane	630-20-6	0.0%	5
1,4-Dinitrobenzene	100-25-4	0.0%	5
1,4-Dioxane	123-91-1	0.0%	5

Name	CAS Number	Detection Frequency (%)	Category
2,3,4,6-Tetrachlorophenol	58-90-2	0.0%	5
2,4,5-Trichlorophenoxyacetic acid/2,4,5-T	93-76-5	0.0%	5
2,4-Dichlorophenol	120-83-2	0.0%	5
2,4-Dimethyl phenol	105-67-9	0.0%	5
2,4-Dimethylaniline (2,4-xylidine)	95-68-1	0.0%	5
2-Chloronaphthalene	91-58-7	0.0%	5
2-sec-Butyl-4,6-dinitrophenol/Dinoseb	88-85-7	0.0%	5
4-Chloroaniline	106-47-8	0.0%	5
Acenaphthylene	208-96-8	0.0%	5
Acetophenone	98-86-2	0.0%	5
Aldrin	309-00-2	0.0%	5
alpha-BHC	319-84-6	0.0%	5
beta-BHC	319-85-7	0.0%	5
bis(2-Chloroethoxy)methane	111-91-1	0.0%	5
bis(2-Chloroethyl)ether	111-44-4	0.0%	5
delta-BHC	319-86-8	0.0%	5
Dieldrin	60-57-1	0.0%	5
Dimethyl phthalate	131-11-3	0.0%	5
gamma-BHC	58-89-9	0.0%	5
Heptachlor epoxide	1024-57-3	0.0%	5
p-Cresidine	120-71-8	0.0%	5

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