

Greenpeace Research Laboratories Analytical Results 2022-02

Provisional screening of a sample of untreated landfill leachate for metals and organic contaminants

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Introduction

A single sample of aqueous liquid waste, reported to have been collected in December 2021 from “leachate well number 8” within the boundaries of the Walleys Quarry landfill in Newcastle-under-Lyme (UK), was received by our laboratories for analysis on 7th January 2022. The sample, measuring approximately 300 ml and being dark brown in colour, had been collected and stored in a washed and rinsed PET soft drinks bottle, and was delivered to our laboratory in this container. On receipt, the sample was assigned the unique sample code NGP22001 and stored in the dark at 4 Celsius until analysis.

Note that because of the ways in which this sample had been collected and stored, the results of the analyses conducted in our laboratory and reported below must be treated strictly as indicative only, in order to guide any further investigations to verify results, and as such must not be used as evidence or in any public communications.

Materials & Methods

Following gentle inversion to ensure homogeneity of the sample, sub-samples were taken to enable a range of forensic analytical screening techniques to be applied, including:

- quantitative analysis for metals using ICP-MS following acid digest
- qualitative screening for volatile organic contaminants using headspace GC-MS,
- qualitative GC-MS screening for semivolatile organic contaminants following sample preparation using a combination of solid-phase extraction (SPE) techniques (Autotrace, HiSorb) and
- LC-MS screening for a range of pesticides (both quantitative and qualitative) following solid phase extraction.

Further details of the methods for each type of analysis are set out in Annex I

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Results

What follows is a brief description of the results obtained from each of the analyses outline above, with brief comparisons where applicable to results reported by ALS Environmental in their report dated 19 July 2016 given analytical results for earlier leachate samples collected from this landfill site. Such comparisons are included on an indicative basis only, recognising that we cannot be certain that the most recent leachate sample analysed in our laboratory was collected from the same locations or in the same way as those previous samples.

Metals

Concentrations for a range of metals (including some toxic heavy metals) are shown in Table 1 below.

For each of the metals and metalloids analysed, the concentration in the filtered sample was very similar to that in the whole, unfiltered, sample, indicating that these analytes were present almost exclusively in dissolved forms within the sample. For the majority of metals and metalloids analysed, the concentration of each was notably higher than concentrations commonly found in uncontaminated surface water and groundwater (Flem *et al.* 2018), but not at concentrations in excess of those that might be expected in a municipal landfill leachate, especially one sampled before any final treatment is applied before discharge.

For the majority of these analytes, the total concentration in the whole sample was similar to those found in samples of leachate collected from this site and analysed in 2016 by an external laboratory (ALS Environmental), with the concentration being within a factor of two of the 2016 concentrations.

Exceptions to this included molybdenum, which was found in the most recent sample at approximately 4 times the concentrations that were found in the samples analysed in 2016, as well as antimony (3-8 times the 2016 concentrations) and tin (2-3 times the 2016 concentrations). Conversely, the elements calcium, copper and zinc were present at somewhat lower concentrations in the most recent sample than those reported in 2016.

Metal/metalloid		Filtered	Whole
Antimony	Sb	108	106
Arsenic	As	143	141
Barium	Ba	981	951
Beryllium	Be	<0.2	<0.2
Boron	B	62500	62200
Cadmium	Cd	0.81	0.85
Calcium	Ca	22900	23100
Chromium (total)	Cr	671	655
Chromium (hexavalent)	Cr (VI)	<60	-
Cobalt	Co	33.1	32.2

Copper	Cu	5.3	9
Iron	Fe	692	839
Lead	Pb	2.6	3.7
Magnesium	Mg	112000	111000
Manganese	Mn	621	622
Mercury	Hg	<0.5	<0.5
Molybdenum	Mo	24.6	24.8
Nickel	Ni	182	171
Potassium	K	609000	623000
Selenium	Se	3	3
Sodium	Na	1910000	1980000
Strontium	Sr	2010	1960
Thorium	Th	<0.1	<0.1
Tin	Sn	50.8	52
Uranium	U	0.4	0.4
Vanadium	V	117	110
Zinc	Zn	31	38

Table 1: Concentrations of metals and metalloids ($\mu\text{g/l}$) in the filtered and the whole, unfiltered, sample

Volatile and semi-volatile organics (VOCs and sVOCs)

A complete list of those compounds (volatile and semi-volatile) that were recovered from the sample using a variety of GC-MS techniques is listed in Annex 2. A total of 138 individual organic compounds were isolated from the sample using a combination of headspace, solid phase desorption and liquid injection GC-MS, of which 108 compounds (78%) could be identified to a high degree of confidence (>90% match quality based on a combination of automated searching against spectral libraries and expert interpretation). This is a relatively high proportion of the total number of compounds isolated from a leachate sample containing a complex mixture of organic chemicals. The remaining 30 compounds could not be identified to a sufficient degree of reliability to be listed.

In most cases, the compounds identified could be considered to be typical for leachates arising from municipal landfills, including a variety of organic acids, alcohols, benzene-derivatives and phenols. Similar ranges of contaminants have been reported in many previous studies of leachate from municipal waste landfills from around the world (e.g. Paxéus 2000, Beldean-Galea *et al.* 2017).

Among those commonly reported compounds also found in the current sample are some that derive from plants and other natural organic materials as they break down, including a variety of terpenoids such as verbanone, camphor, thujanone and eucalyptol. Others are synthetic compounds manufactured for use as plasticisers or antioxidants in plastics (e.g. phthalate esters, 3,5-di-tert-butyl-4-hydroxyphenylpropionic

acid), or as solvents in personal care products (e.g. dihydrofuranone). A number of organophosphate flame retardants were also present in the leachate (e.g. tributyl phosphate and triethyl phosphate), compounds that have also been reported in other studies of landfill leachate and which probably arise from their use in textiles or plastics. The strongly odorous compound trimethylsilanol is another substance frequently reported in both biogas and leachate from landfills, and is thought to derive from products such as silicone rubbers and sealants.

Two less commonly reported synthetic compounds found in this sample were benzenecetic acid, an ingredient in a range of industrial cleaning and waxing products, and N-butyl benzenesulphonamide (NBBS, a suspected neurotoxic substance), used as a plasticizer in a range of polyacetals, polyamides, polysulphones and polycarbonates, though which can also be generated naturally by some bacteria (Rider *et al.* 2012). Also present were residues of the hormone-disrupting chemicals bisphenol-A and its fluorinated derivative bisphenol-AF. All of these compounds could arise from consumer products disposed of to the landfill over time, but could also derive from wastes of industrial origin. Likewise, residues of the pain relief drug ibuprofen could arise from either domestic or industrial sources.

Some of the other less common compounds identified in the current sample may be even more suggestive of the disposal at the site of wastes from industrial origins, including the compound 2-chloro-3,4-diphenyl benzofuro[2,3-b]pyridine (used in the pharmaceutical industry), the industrial solvents 1-butyl pyrrolidone, N,N'-dimethyl cyclohexanimine and 2,6-dimethyl-4-heptanone, and a chemical used in the manufacture of polyurethane, namely tributylamine.

Perhaps of even greater concern is the presence of detectable residues of the toxic organochlorine chemicals 1,1-(chloromethylene)*bis* benzene (an initiator used in the manufacture of polystyrene) and dichloroaniline, a synthetic chemical used in industrial dyeing operations, as well as triethylamine (used as an auxiliary chemical in textile dyeing) and a range of substituted pyridines typically used as intermediates in the pharmaceutical industry.

The work conducted by ALS Ltd on leachate samples collected from the same site in 2016 did include targeted analysis for some specific volatile and semi-volatile organic compounds, including the toluene, ethylbenzene and xylene residues also found in the more recent sample in our laboratory (among those compounds listed in Annex 2). However, the majority of other contaminants which we have been able to identify in the 2021 sample using our wide qualitative screening techniques would not have been discovered through the more targeted analysis applied by ALS in order to detect and quantify a more limited list of target analytes. Direct comparison of our data with those from the leachates analysed in 2016 is therefore not possible, though our research demonstrates the additional forensic power of GC-MS screening in scan mode to detect a wide array of compounds, some of them quite toxic, which might otherwise be missed.

Pesticides

In addition to the chemicals identified in the VOC and sVOC screening described above, LC-MS analysis confirmed the presence of residues of a total of 6 pesticide active ingredients in the leachate sample, as

listed in table 2 below, along with their determined concentrations. Carbendazim is most commonly used as a fungicide, as is the case for Propiconazole and Tebuconazole, while the other three compounds identified in the sample are herbicides. It cannot be determined from these results whether the presence of these residues relates to their leaching from wastes or their use on or around the landfill site in order to control weeds and fungal growth. The concentration of bentazone in this sample was particularly high, perhaps suggestive of local and relatively recent application in the vicinity, though the possibility that the compound arose from the disposal of herbicide-containing wastes at the site cannot be ruled out on this basis.

Compound name	Neutral Mass	Formula	concentration in sample (ng/L)
Carbendazim	191.0694	C ₉ H ₉ N ₃ O ₂	23.6
Chloridazon	221.0355	C ₁₀ H ₈ ClN ₃ O	187.0
Napropamide	271.1572	C ₁₇ H ₂₁ NO ₂	69.7
Propiconazole	341.0697	C ₁₅ H ₁₇ Cl ₂ N ₃ O ₂	284.6
Tebuconazole	307.1451	C ₁₆ H ₂₂ ClN ₃ O	268.2
Bentazone	240.0568	C ₁₀ H ₁₂ N ₂ O ₃ S	18 549=18.54 ug/L

Table 2: Pesticide active ingredients that could be identified and quantified by HPLC-MS in the sample

In leachate samples analysed in 2016 by an external laboratory (ALS Environmental), residues of the pesticides Dichlobenil, MCPA and Mecoprop were identified. Interestingly, none of those pesticides could be reliably confirmed as being present in the sample we received for analysis. Residues of Dichlobenil would be unlikely to have been detected using the LC-MS system employed in this analysis. Mecoprop would be, but is not an active ingredient for which we have an appropriate standard in order to validate the method. Residues of the herbicide MCPA would also have been detectable and quantifiable using our validated HPLC-MS method, if such residues had been present. In the case of Mecoprop, manual searches of the total ion chromatograms (TIC) obtained for the sample suggest that small traces of Mecoprop may have been present in the most recent leachate sample, though further investigations would be needed to confirm this.

Concluding remarks

While it is not possible to draw any definitive conclusions about the specific origins of any of the chemicals identified through this analysis, the presence of a such a diverse array of chemical contaminants, including some known to be used in industrial chemistry applications and some known to be highly toxic, is clearly a cause for concern and a justification for further investigation, including into the origins of the wastes on site. The leachate arising from landfills can effectively integrate pollutants from a range of wastes disposed within those sites over their period of operation, especially given that some of the contaminants identified are persistent chemicals that are resistant to biodegradation.

It should be noted that the sample we received for analysis was collected prior to any final treatment process, such that it remains to be determined if any such treatment could be effective in destroying or removing the chemicals of concern from such a complex mix of contaminants.

It should also be noted that the sample we analysed had been collected in a bottle that had previously contained a soft drink and that, however thorough the cleaning process applied before it was used to collect the leachate sample, the possibility cannot be ruled out that at least a fraction of the contaminants identified through our analyses (the phthalate esters, for example) may have arisen as a result of leaching from the plastic bottle into the leachate sample during storage. Any subsequent samples for analysis should be collected into glass bottles that have been pre-cleaned using an acid and solvent wash procedure in order to avoid the potential for cross contamination.

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References

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Annex 1: details of analytical methods applied

Metals

A portion of the homogenised sample was acidified by the addition of concentrated nitric acid (5% v/v) and hydrochloric acid (0.5% v/v). Separately, another portion of the homogenised sample was filtered through a 0.45 micron filter and then acidified in the same way to enable determination of dissolved metal concentrations. 25 ml of each acidified sample was digested firstly overnight at room temperature, then using microwave-assisted digestion with a CEM MARS Xpress system, with a temperature ramp to 180°C over 20 minutes followed by holding at 180°C for a further 20 minutes. Cooled digests were filtered and made up to 25 ml with deionised water. For quality control purposes, a blank sample, and a mixed metal solution of 80 µg/l for each metal, other than mercury at 4 µg/l, were digested in an identical manner.

Sample digests were analysed by Inductively Coupled Plasma Mass Spectrometry (ICP-MS) using an Agilent 7900 Spectrometer utilising a collision cell with helium as the collision gas to minimise polyatomic interferences. Multi-element standards, matrix matched to the samples, at concentrations of 1, 10, 100 and 1000 µg/l respectively, other than for mercury (1, 2, 5, 20 µg/l respectively) were used for instrument calibration. Calibration was validated by the analysis of quality control standards at 80 µg/l and 800 µg/l (4 µg/l and 16 µg/l for mercury) prepared in an identical manner but from different reagent stocks to the instrument calibration standards. Analysis employed in-line addition of an internal standard mix at 100 µg/l (Scandium, Germanium, Yttrium, Indium and Terbium). Any sample exceeding the calibration range was diluted accordingly, in duplicate, and re-analysed.

The concentration of hexavalent chromium (VI) was determined colorimetric for a portion of the sample filtered through a 0.45 micron filter. A freshly prepared solution of 1,5-diphenylcarbazide (0.5 ml) was added to 9.5 ml of the filtered sample. The solution was mixed and allowed to stand for 10 minutes to allow full colour development. Concentrations were determined using a spectrophotometer at 540 nm, correcting with a blank prepared from deionised water, and using calibration standards freshly prepared from potassium dichromate at concentrations of 0, 20, 100 and 300 mg/l respectively. For quality control, a blank deionised water sample and a quality control solution of 150 µg/l Cr (VI) were analysed separately, as well as a separate portion of the sample spiked with the addition of 300 µg/l Cr (VI).

Volatile organics (VOCs) using headspace GC-MS

Shortly after arrival at our laboratory, 3 x 10ml of undiluted sample were transferred to clean glass 20ml headspace vials and capped, before storage in the dark at 4 Celsius prior to analysis for volatile organic compounds (VOCs). Headspace GC-MS analysis was performed using a Markes Centri sample introduction system equipped with a headspace tool, linked to an Agilent 7980B gas chromatograph and Agilent 5977A mass spectrometer. Samples were heated to 60 C for 10 minutes with agitation in order to increase the partitioning of volatile (low boiling point) organic compounds from the samples into the headspace of the vial, before a 5ml headspace sample was withdrawn and introduced into the injection port of the Centri system, which was held at 250 C. VOCs were captured and concentrated on a cold trap,

which was subsequently desorbed up to a temperature of 300 C and the analytes carried through a heated transfer line to the GC-MS. Several deionised water samples were used as procedure blanks.

Compounds were separated in the GC oven using a Restek Rxi-624 Sil MS column (30m, 0.25 i.d., 1.4µm coating), held initially at 40 C for 4 minutes, then ramped at 15 C/min to 240 C, which was held for 10 mins before finally ramping at 50 C/min to 260 C for 2 minutes to ensure that the column was clean before the next sample. Separated compounds were carried into the mass spectrometer operating in SCAN mode in order to conduct a qualitative forensic screen for as wide a range of VOCs as possible, using a mass/charge ratio range of 35 to 450. Individual compounds were identified as far as possible by spectral matching against two MS compounds libraries (Wiley 10N11 and NIST 11), with expert interpretation to check for match quality. Only those compounds which could be identified to greater than 90% match quality, and which could not be detected in the deionised water procedural blanks, have been reported.

Semi-volatile organics (sVOCs) using solid phase extraction (SPE) and liquid injection GC-MS

GCMS Scan Extraction

Due to the amount of sample provided and its nature (density and odour), 100mL of the sample were diluted into 400mL of DI water. A blank sample, composed of 500mL DI water, was extracted along with the analysed sample. 10 µg of deuterated naphthalene were added as an Internal Standard (IS) to sample and blank.

Both samples were prepared using solid phase extraction technique with Dionex AutoTrace workstation. The eluting solvents were ethyl acetate followed by a mixture of pentane and toluene 95:5. The 10mL extracts resulted were divided into two 5 mL aliquots and treated with different cleaning techniques:

5mL were submitted to DSPE (Disperse Solid Phase Extraction) technique, based on drying and cleaning active agents. 1mL of the resulting supernatant was vialled, ready for injection*.

5mL were subjected to florisil cleaning procedure, the extract concentrated to 0.5mL and then rinsed and reconstituted to a 1mL in pentane.

Obtained extracts were analysed with GC/MS.

*This extract was supplied by Ildiko, which means that the sample was acidified before extraction and the extract was based in methanol.

GC/MS analysis

For the total organic compounds screening, samples were analysed using an Agilent 6890 Series II GC with Restek Rtx-17Sil column (30m, 0.25mm ID, 0.25 µm film thickness) linked to an Agilent 5975B Inert MSD operated in EI mode and interfaced with an Agilent Enhanced Chem Station data system. Total Ion chromatograms (TIC) and Selected Ion Monitoring (SIM) chromatograms were obtained. The GC oven temperature program employed was as follows: an initial temperature of 40°C, raised to 260°C at

10°C/min, then to 295°C at 50°C/min (held for 10 min), then to 325°C at 50°C/min (held for 25 min), finally raised to 330°C at 50°C/min (held for 1 min). The carrier gas was helium, supplied at 1ml/min.

The identification of the compounds was carried out by matching spectra obtained during analysis against both the Wiley W10N11 and Pesticides Libraries in conjunction with the data resulted from the SIM mode. In addition, the presence of chemicals in certain chemical groups was further investigated using other techniques available in ChemStation software (e.g., peak purity and specific ion extraction).

Additional semi-volatile organics (sVOCs) using HiSorb solid phase extraction (SPE) probes and thermal desorption GC-MS

As a further check for the presence of semivolatile organic compounds (sVOCs), an additional sub-sample of 5ml was diluted with 5 ml of deionised water in a clean 20ml glass vial, and analysed using solid phase extraction/thermal desorption GC-MS. The diluted sample was heated and agitated at 60 C for 5 minutes before insertion of a HiSorb PDMS solid phase extraction probe and heating and agitation for a further 30 minutes. The HiSorb probe was then removed from the sample, washed with deionised water, dried in a stream of nitrogen and inserted into the injection port of the Centri sample introduction system held at a temperature of 250 C. sVOCs that had adhered to the PDMS surface of the probe were desorbed and concentrated onto a cold trap, which was then heated to 300 C in order to carry those compounds through the heated transfer line and on to the GC-MS.

As for the VOC analysis outlined above, compounds were separated in the GC oven using a Restek Rxi-624 Sil MS column (30m, 0.25 i.d., 1.4um coating), held initially at 40 C for 4 minutes, then ramped at 15 C/min to 240 C, which was held for 10 mins before finally ramping at 50 C/min to 260 C for 2 minutes to ensure that the column was clean before the next sample. Separated compounds were carried into the mass spectrometer operating in SCAN mode in order to conduct a qualitative forensic screen for as wide a range of VOCs as possible, using a mass/charge ratio range of 35 to 450. Individual compounds were identified as far as possible by spectral matching against two MS compounds libraries (Wiley 10N11 and NIST 11), with expert interpretation to check for match quality. Only those compounds which could be identified to greater than 90% match quality, and which could not be detected in the deionised water procedural blanks, have been reported.

Pesticides using solid phase extraction (SPE) and LC-MS

Sample preparation

Sample was taken out from the fridge and stored at ambient temperature for 30 min before the analytical process. 1x 100mL leachate liquid was precisely measured and diluted with 100mL DI water. The diluted sample (200mL) was filtered through 0.7um glass fibre filter paper and acidified with formic acid to pH=3.15 and was extracted using an Autotrace SPE system.

NOTE: initial pH= 7.68. During acidification foaming process occurred

Short description of the autotrace (AT) solid phase extraction (SPE) technique (method: number 13, pesticide):

- Oasis HLB sorbent was conditioned (1st methanol, 2nd pH=3 distilled water)
- 200 mL of each filtered and acidified (pH=3) diluted sample were loaded to the sorbent
- drying step with N₂ flow
- HLB sorbent was eluted with 10 mL of methanol
- 10 mL methanol volume was reduced to 1 mL

Additional clean was needed as fluffy/flaky precipitation was in the autrace extract, therefore d-SPE clean was done on 5mL AT extract with Thermo d-SPE tube (750mg MgSO₄, 250mg PSA, 250mg, Carbon, 250mg C18). 1 min handshake and 1 min vortex were followed by a centrifuge separation (5 min at 3000rpm). Supernatant was ready for LC-MS injection.

Samples were stored in the fridge till the LC-MS analysis.

HPLC-MS measurements:

The extracted samples were analysed for [251 pesticides](#); semi-quantitative determination was carried out using external calibration standards. Short description of the liquid chromatographic (LC) technique coupled with mass spectrometry (MS) method (LC-ESI-Q-Orbitrap-MS):

- Gradient chromatographic conditions (with eluents “A”= water+2% methanol+0.1% formic acid+5mM ammonium formate, “B”= methanol+2%water+0.1% formic acid+5mM ammonium formate)
- Separation was carried out on Accucore aQ C18 column
- MS analysis was carried out both positive and negative ionisation mode
Mater methods contains all measurement parameters:

Pesticide Confirmation POS CM7 IK_10uL and Pesticide Confirmation NEG CM7 IK

NB: for determined pesticide concentration: calibration curve coefficients of determination (R^2) were all between: 0.89-0.99.

Annex 2: full list of volatile (VOC) and semi-volatile (sVOC) organic compounds identified in leachate sample NGP22001

Number of compounds isolated: 138

Compounds identified to better than 90%:

In total ion chromatogram (TIC)

CAS#	Name
000000-00-0	(+)-Neoisomenthol
000464-49-3	(+)-2-Bornanone (Synonym: dextro-Camphor)
000000-00-0	(S)-(-)-Verbanone
000098-55-5	.alpha.-Terpineol
000470-08-6	.beta. Fenchyl alcohol
000092-52-4	1,1'-Biphenyl
000085-68-7	1,2-Benzenedicarboxylic acid, butyl benzyl ester
000083-32-9	1,2-Dihydro-acenaphthylene (Synonym: Acenaphthene)
002094-97-5	1,3-Oxathiolane
000934-34-9	2(3H)-Benzothiazolone
000096-48-0	2(3H)-Furanone, dihydro-
000565-80-0	2,4-Dimethyl-3-pentanone
000719-22-2	2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-
000000-00-0	2-chloro-3,4-diphenyl benzofuro[2,3-b]pyridine
015679-12-6	2-Ethyl-4-methylthiazole
000470-82-6	2-Oxabicyclo[2.2.2]octane, 1,3,3-trimethyl- (Synonyms: Cineole, Eucalyptol)
003470-98-2	2-Pyrrolidinone, 1-butyl-
000000-00-0	2-(((1,1-Bis(methylthio)-2-methyl-1,3-pentadienylidene))-6- methoxy-1-tetralone
020170-32-5	3,5-Di-tert-butyl-4-hydroxyphenylpropionic acid
001125-12-8	1-Isopropyl-4-methylbicyclo[3.1.0]hexan-3-one (Synonym: 3-Thujanone)
037275-49-3	4,7-Methano-1H-indenol, hexahydro-
014888-58-5	4,7-Methano-5h-inden-5-one, 3,3a,4,6,7,7a-hexahydro-
000108-83-8	4-Heptanone, 2,6-dimethyl-
000586-82-3	4-Isopropyl-1-methyl-3-cyclohexen-1-ol
000470-67-7	7-Oxabicyclo[2.2.1]heptane, 1-methyl-4-(1-methylethyl)-
000086-73-7	9H-Fluorene
006566-19-4	10,18-Bisnorabieta-5,7,9(10),11,13-pentaene
000098-86-2	Acetophenone
038861-78-8	Acetophenone, 4-isobutyl-
000102-82-9	Amine, tributyl-
000120-12-7	Anthracene
000947-04-6	Azacyclotridecan-2-one
000103-82-2	Benzeneacetic acid
000134-62-3	Benzamide, N,N-diethyl-3-methyl- (Synonym: DEET)

000554-00-7	Benzenamine, 2,4-dichloro-
001197-01-9	Benzenemethanol, .alpha.,.alpha.,4-trimethyl-
000617-94-7	Benzenemethanol, .alpha.,.alpha.-dimethyl-
000501-52-0	Benzenepropanoic acid
003622-84-2	Benzenesulfonamide, N-butyl-
001077-56-1	Benzenesulfonamide, N-ethyl-2-methyl-
000080-39-7	Benzenesulfonamide, N-ethyl-4-methyl-
000090-99-3	Benzene, 1,1'-(chloromethylene)bis-
002094-99-7	Benzene, 1-(1-isocyanato-1-methylethyl)-3-(1-methylethenyl)-
000098-83-9	Benzene, (1-methylethenyl)-
000526-73-8	Benzene, 1,2,3-trimethyl-
000095-63-6	Benzene, 1,2,4-trimethyl-
000108-38-3	Benzene, 1,3-dimethyl- (Synonym: Xylene)
000622-96-8	Benzene, 1-ethyl-4-methyl-
000100-41-4	Benzene, ethyl-
000108-83-3	Benzene, methyl- (Synonym: Toluene)
000065-85-0	Benzoic acid
000480-63-7	Benzoic acid, 2,4,6-trimethyl-
000119-61-9	Benzophenone
001195-79-5	Bicyclo[2.2.1]heptan-2-one, 1,3,3-trimethyl-
000076-22-2	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl- (Synonym: dextro-levo-Camphor)
000128-37-0	Butylated hydroxy toluene
000075-15-0	Carbon disulphide
000098-94-2	Cyclohexanamine, N,N-dimethyl-
000100-60-7	Cyclohexanamine, N-methyl-
007322-63-6	Cyclohexanemethanol, .alpha.,.alpha.,4-trimethyl-, cis-
000000-00-0	Cyclohexanol
000089-80-5	Cyclohexanone, 5-methyl-2-(1-methylethyl)-, trans-
062238-12-4	Decane, 2,3,6-trimethyl-
000057-10-3	Hexadecanoic acid
000149-57-5	Hexanoic acid, 2-ethyl-
003302-10-1	Hexanoic acid, 3,5,5-trimethyl-
000119-84-6	Hydrocoumarin
015687-27-1	Ibuprofen
026444-19-9	Ethanone, 1-(methylphenyl)-
000496-11-7	Indane
000091-20-3	Naphthalene
000119-61-9	Methanone, diphenyl-
000124-26-5	Octadecanamide
000085-01-8	Phenanthrene
000108-95-2	Phenol
000088-69-7	Phenol, 2-(1-methylethyl)-
000096-76-4	Phenol, 2,4-bis(1,1-dimethylethyl)-
000088-69-7	Phenol, 2-(1-methylethyl)-
000620-17-7	Phenol, 3-ethyl-
000621-27-2	Phenol, 3-propyl-
000080-05-7	Phenol, 4,4'-(1-methylethylidene)bis- (Synonym: Bisphenol A)

001478-61-1 hexafluoride)	4,4'-(Hexafluoroisopropylidene)diphenol (Synonym: Bisphenol A
000599-64-4	Phenol, 4-(1-methyl-1-phenylethyl)-
000099-89-8	Phenol, 4-(1-methylethyl)-
000000-00-0	Phenol, 4-[(4-Fluorophenyl)methyl]-
000106-44-5	Phenol, 4-methyl-
004286-23-1	Phenol, p-isopropenyl-
000098-54-4	Phenol, p-tert-butyl-
000126-73-8	Phosphoric acid, tributyl ester
000078-40-0	Phosphoric acid, triethyl ester
000513-02-0	Phosphoric acid, triisopropyl ester
066735-04-4	Propanoic acid, 2-methyl-3-[4-t-butyl]phenyl-
001124-11-4	Pyrazine, 2,3,5,6-tetramethyl-
000108-75-8	Pyridine, 2,4,6-trimethyl-
000000-00-0	Pyridine, 2-ethyl-
000109-06-8	Pyridine, 2-methyl-
000536-78-7	Pyridine, 3-ethyl-
000108-99-6	Pyridine, 3-methyl-
000000-00-0	Pyrimidine, 4-ethyl-2,5,6-trimethyl-
000108-88-3	Toluene
000000-00-0	Tricyclo[5.2.1.0(2,6)]dec-4-en-8-one
000121-44-8	Triethylamine
001066-40-6	Trimethylsilanol
000106-42-3	p-Xylene

In selective ion monitoring mode (SIM)

CAS#	Name
000084-66-2	1,2-Benzenedicarboxylic acid, diethyl ester
000084-69-5	1,2-Benzenedicarboxylic acid, diisobutyl ester
000084-74-2	1,2-Benzenedicarboxylic acid, dibutyl ester
000206-44-0	Fluoranthene
000129-00-0	Pyrene