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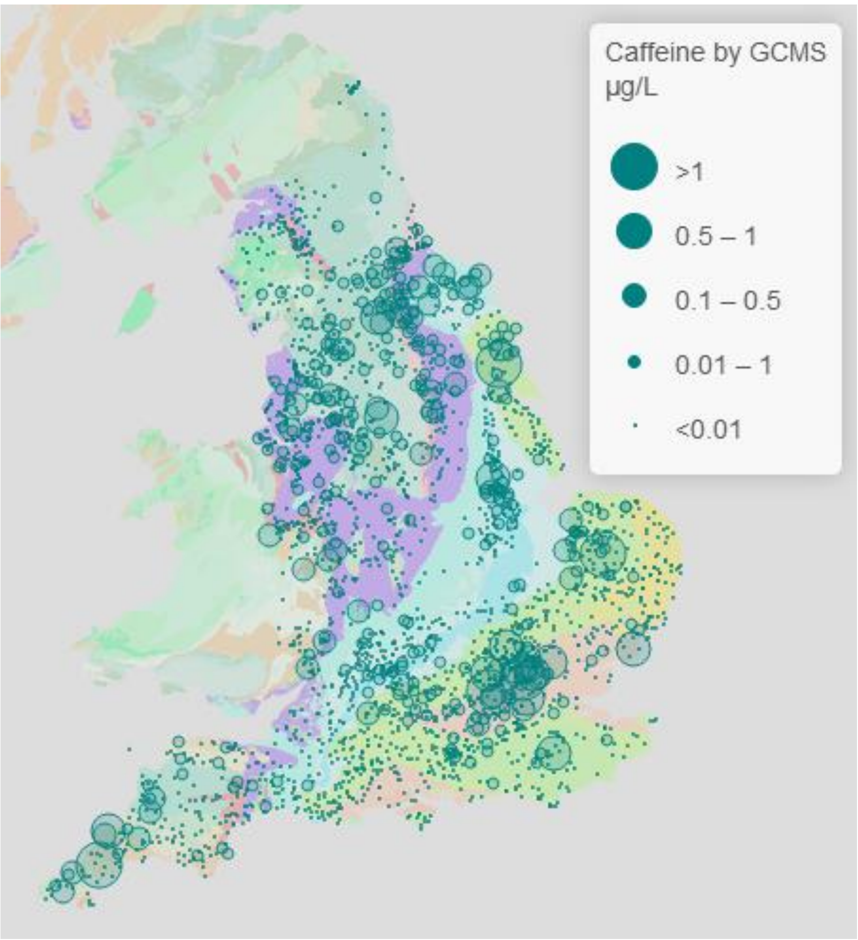
Micro-organic contaminants in groundwater in England: summary results from the Environment Agency LC-MS and GC-MS screening data

Groundwater Programme

Open Report OR/18/052



BRITISH GEOLOGICAL SURVEY

GROUNDWATER PROGRAMME

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Micro-organic contaminants in groundwater in England: summary results from the Environment Agency LC-MS and GC-MS screening data

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Distribution of concentrations of the insect repellent Caffeine in groundwater

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Foreword

This report is the published product of a study by the British Geological Survey (BGS) ‘Emerging substances in groundwater’ that was undertaken for the Environment Agency. The focus of this work was to undertake a rigorous assessment of summary statistics for the top 50 most frequently detected compounds in both the LC-MS and GC-MS groundwater screen data.

Acknowledgements

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Summary

This report describes the results from summarising Environment Agency groundwater monitoring data for trace organic compounds from two targeted scanning semi-quantitative methods. The Gas chromatography mass spectroscopy (GC-MS)[1] method has been regularly used for groundwater samples since 2001 and provides semi-quantitative data for neutral, hydrophobic compounds amenable to separation by gas chromatography. These include a wide range of industrial compounds, halogenated solvents and trihalomethanes (THMs), plasticisers and pesticides, with relatively few pharmaceuticals. The Ultra-High-Definition (UHD) Accurate-Mass Quadrupole Time-of-Flight (Q-TOF) liquid chromatography-mass spectrometry (LC-MS) method has been used from 2012 onwards for groundwater samples and complements the GC-MS method by providing data on polar, more hydrophilic compounds including many pesticides and pharmaceuticals, as well as perfluorinated compounds (PFCs). Some compounds, such as atrazine, are detected by both methods.

The aim of this project was to analyse Environment Agency GC-MS (2009-2017) and LC-MS (2016-2017) semi-quantitative (targeted) screening data for emerging contaminants in groundwater and to produce summary statistics, selected charts, maps and a summary report. When interpreting the results of this report additional caution is required because of the semi-quantitative nature of these screening methods and also because these screening methods are so sensitive unforeseen sample contamination can be an issue.

The results from the GC-MS method showed that out of the top 50 most frequently detected compounds 13 were industrial compounds, 8 were pesticides and their transformation products, 9 were pharmaceuticals, personal care products or lifestyle compounds (PPCL), 8 were polyaromatic hydrocarbons, 7 were halogenated solvents and 5 were plasticisers. Limits of quantification for this method are predominantly 0.01 μg/L with higher limits for four compounds, the industrial compound 2,4,7,9-Tetramethyl-5-decyne-4,7-diol (TMDD), the food additive Butylated hydroxytoluene (BHT), and the plasticisers benzenesulfonamide, N-butyl (BBSA) and Bis(2-ethylhexyl)phthalate DEHP.

The results were similar to those reported in 2016 but with some key differences:

- There were fewer overall detections due to the removal of non-GC-MS specific data from the analysis: this was most obvious for the halogenated solvents
- Some compounds were less prominent possibly due to analytical methodology improvements with the reduction in the number of false positives. An example of this would be caffeine
- Some new compounds appeared in the top 50 most frequently detected compounds, e.g. butanedioic acid, and dimethyl ester (dimethyl succinate)

Ordering the results using maximum concentrations gives a very different set of compounds with the plasticiser BBSA having the highest maximum concentration.

For the LC-MS data 36 of the top 50 most frequently detected compounds were pesticides, with others being 8 PPCL and 6 industrial compounds. Ordering the results by maximum concentration indicates that 3 out of 5 of the highest concentrations were for the PPCLs clopidol, sucralose and pentobarbital.

The quantification limits for the LC-MS method which are at 0.001 μg/L are predominantly an order of magnitude lower than for the GC-MS, increasing for perfluorinated compounds and also for the PPCLs sucralose, sulphanilamide and sulfamethoxazole, and the pesticides boscalid,

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[1] Please see the glossary for expansions of acronyms

trietazine and mecoprop. The percentage of samples with positive detections is much higher, 5-65%, for the LC-MS data compared to typically 1-2% for the GC-MS.

The ranges of LODs for Environment Agency quantitative analytical suites are of a similar order of magnitude to the LC-MS method with higher limits for PAHs and difficult compounds, such as the pesticides chlormequat and glyphosate which can only be analysed with quantitative methods.

Both the target GC-MS and the LC-MS methods detect a much wider range of compounds than the Environment Agency standard suites (also using GC-MS and LC-MS) currently cover.

1 Introduction

A large variety of organic compounds are used in huge quantities for a range of purposes (e.g. manufacturing, food production, healthcare). Some of these have been identified as micro-organic (MO) (low concentration) contaminants in the environment. Interest in the occurrence of MO contaminants in the water environment continues to grow, and more sensitive analytical methods have led to an increasing number of these substances being detected in groundwater. The data analysis carried out as part of this project will allow the Environment Agency to: better understand the risks to groundwater from emerging substances, answer questions from key stakeholders, feed into a future chemicals strategy, contribute to the EU Groundwater Watch List work and contribute to the Government's 25 Year Environment Plan.

This report describes the results from summarising Environment Agency groundwater monitoring data for trace organic compounds from two targeted scanning semi-quantitative methods. The GC-MS method has been regularly used for groundwater since 2001 and provides semi-quantitative data for neutral, hydrophobic compounds amenable to separation by gas chromatography. These include a wide range of industrial compounds, halogenated solvents and trihalomethanes (THMs), plasticisers and pesticides, with relatively few pharmaceuticals. The LC-MS method has been more recently introduced and complements the GC-MS method by providing data on polar, more hydrophilic compounds including many pesticides and pharmaceuticals, as well as perfluorinated compounds (PFCs). Some compounds, such as atrazine, are detected by both methods.

The aim of this project is to analyse Environment Agency GC-MS and LC-MS semi-quantitative screening data for emerging contaminants in groundwater and to produce summary statistics, charts and a summary report.

These objectives were addressed by a series of tasks:

- Development of a methodology for processing the raw data from the Environment Agency's Water Information Management System (WIMS) to deal with data entry errors and produce a "clean" database (Chapter 2)
- Development of a statistical procedure (Chapter 2)
- Visualisation of summary results in bar charts (frequency of detection and maximum concentration), box plots, summary tables and spatial plots (Chapter 3)
- Provision of context by commenting on key substances with high frequency of detections and spatial hotspots, comparison with previous studies in the UK and implications for the use of targeted scanning methods compared to quantitative analytical suites (Chapter 4).

The dataset includes data from 63 sites which are not part of the Groundwater Quality Monitoring Network (GWQMN). Some samples may have been intentionally collected from, or close to, known contaminated sites for a specific purpose other than general screening. Such samples could contain relatively high concentrations of contaminants. The remit of this study was to assess all available groundwater data and therefore we have not made a distinction between data collected for different reasons in this analysis.

2 Methods

2.1 DATA SOURCES

The Environment Agency has a statutory responsibility for monitoring the quality of groundwater in England. As part of their monitoring programme, samples for micro-organic compounds are collected and analysed in response to Water Framework Directive and Groundwater Directive requirements, and for State of the Environment reporting. Most of the monitoring points used in this report are from the Environment Agency's Groundwater Quality Monitoring Network. These monitoring points were selected to represent the regional quality of the groundwater. However, there are also a relatively small number of other sites included in the results and some of these could be point source monitoring points. These point source monitoring points could account for some of the maximum concentration values presented in later in this report.

Data we have been provided with (Section 2.2) have come from analyses undertaken by the National Laboratory Service. Targeted GC-MS and LC-MS screening for organic substances was carried out following sample pre-concentration. For the GC-MS method a double liquid-liquid extraction was employed, using acid-neutral dichloromethane, to extract non-polar substances. Oasis® HLB cartridges were used for SPE for the LC-MS method, elution was done using 0.1% Formic acid in methanol/acetonitrile (1:1).

The GC-MS target based (multi-residue) screening method allowed for almost all GC-amenable pesticides as well as hundreds of other organic contaminants to be identified from a single sample, incorporating over 850 substances and including both volatile organic compounds (VOCs) and semi-volatile organic compounds (SVOCs). Chemicals could be identified at concentrations as low as 0.01 µg/L using deconvolution reporting software (DRS).

A LC-MS (Q-TOF) method (e.g. Batt and Aga, 2005) was used to screen for polar organic compounds in each sample. Target compounds for quantification have been analysed in a blank and at a concentration of 0.1 µg/L, the response factor obtained is used to create a single point calibration curve. Estimate of concentration is based on quant ion response and response of the internal standard. Quantification limits are compound specific and are typically between 0.001-0.1 µg/L for the vast majority of compounds. Target compound identification is made by retention time, accurate mass and by isotope distribution patterns (mass, ratio, spacing). The combined results contribute to an overall match score for each substance.

2.2 DATA COLLATION AND PROCESSING

GC-MS and LC-MS data provided to BGS by the EA represents all available groundwater samples analysed as part of EA monitoring activities and the vast majority of data come from the EAs national groundwater quality monitoring network. Data from one-off investigations could also be included and may in some cases could account for high detection frequencies and concentrations, although this has not been investigated as part of this study. This target screening data provides surveillance data on a broad range of substances and complements the dedicated and much smaller EA analytical suites used for monitoring and regulatory purposes (e.g. pesticides and TPs).

2.2.1 GC-MS data

EXISTING BGS DATABASE

BGS was first given access to Environment Agency GC-MS semi-quantitative screening data in 2010. The initial raw dataset contained 17,694 records with monitoring sites in both England and Wales. Additional data was provided in 2012, with an interpretation reported by Manamsa et al., 2016. Data processing included both automated (using queries) and manual data separation (e.g. to extract data where multiple records were presented concatenated into a single record) and cleaning (e.g. correcting CAS numbers). The cleaned data is stored in a Microsoft Access database.

ADDITIONAL RAW GC-MS DATA

The most recent GC-MS data (England only) were provided in October 2017 and appended to the existing BGS database. The recent raw data has fewer data formatting errors than earlier tranches. Data processing was undertaken as described below (Section 2.2.3).

The current version of the BGS database contains 27,283 records (each of which has a unique sample site + sample date + determinand), taken from 7473 samples, and 2465 sites. The BGS database now contains data from samples which were analysed between June 2009 and July 2017.

In general, only detected values were reported, however, 134 records contain a "<" symbol in the "less than" field: in these cases records were converted to below Limit of Detection (LOD), i.e. distinguishable from the blank, by recording "<LOD" in the "value" field.

Three records had a blank "value" field and were excluded from our data analysis.

GC-MS DATA FROM SITES IN WALES

The BGS database includes data from 62 sites in Wales. There are 213 records (unique sample site + sample date + determinand) for Wales (excluding records for the sulphur compound S_8). One of the 213 records reports a "less than" value. This data dates from prior to the formation of Natural Resources Wales in April 2013 (sample dates range from August 2009 to July 2012), and are therefore only a subset of data that exists for Wales.

The Wales data as described above was included in the statistical analysis but excluded from spatial plots. As they comprise less than 1% of the database their inclusion will not have a noticeable impact on the results of the statistical summaries.

2.2.2 LC-MS data

The LC-MS semi-quantitative screen has been introduced more recently and this is the first time that BGS has undertaken an analysis of this data. The data was provided to BGS in October 2017 and covers results between reported from April 2014 to October 2017. There are 4,089 records from 249 samples collected from 109 sites (all in England). No "<" values were recorded in the "less than" field. This method was introduced as a trial in a number of EA Areas and has not been used across the EA groundwater quality-monitoring network in the same way as the GC-MS screen and therefore only data for a subset of monitoring sites is available to date.

2.2.3 Workflow to prepare the GC-MS and LC-MS datasets

The workflow used to prepare the datasets for statistical analysis and spatial plotting is summarised in Figure 2.1. The steps involved were:

1. Additional data (more recent GC-MS and all LC-MS) provided by the Environment Agency for this study was appended to the existing BGS database (in Microsoft Access), using a query to exclude duplicate records.
2. Data cleaning:
    - Manual correction of a small number of records was undertaken where data formatting errors were identified
    - Records where the value field (concentration) was blank were excluded
    - CAS numbers were reformatted where necessary to make them consistent (e.g. removing hyphens)
    - Records reporting concentrations of the sulphur compounds S_8 (CAS number 10544500; cyclooctasulphur) and S_6 (CAS number 13798237; hexathiane) were excluded, as they are not organic compounds
3. The remaining records in the database should be positive detections, however, some records reported '<' in the "less than" field and others had a reported value (concentration) of "0": these were assigned <LOD value for data analysis and reporting purposes

4. The top 50 compounds (ranked by number of detections) were determined for the two screening methods (GC-MS and LC-MS)
5. The data for the top 50 compounds was then exported to Excel. The exported data consisted of a concentration for each (unique site + sampling date) and the dataset was then manually completed by assigning a <LOD value to empty cells (as this is a screening method, all determinands were by default analysed for in each sample).

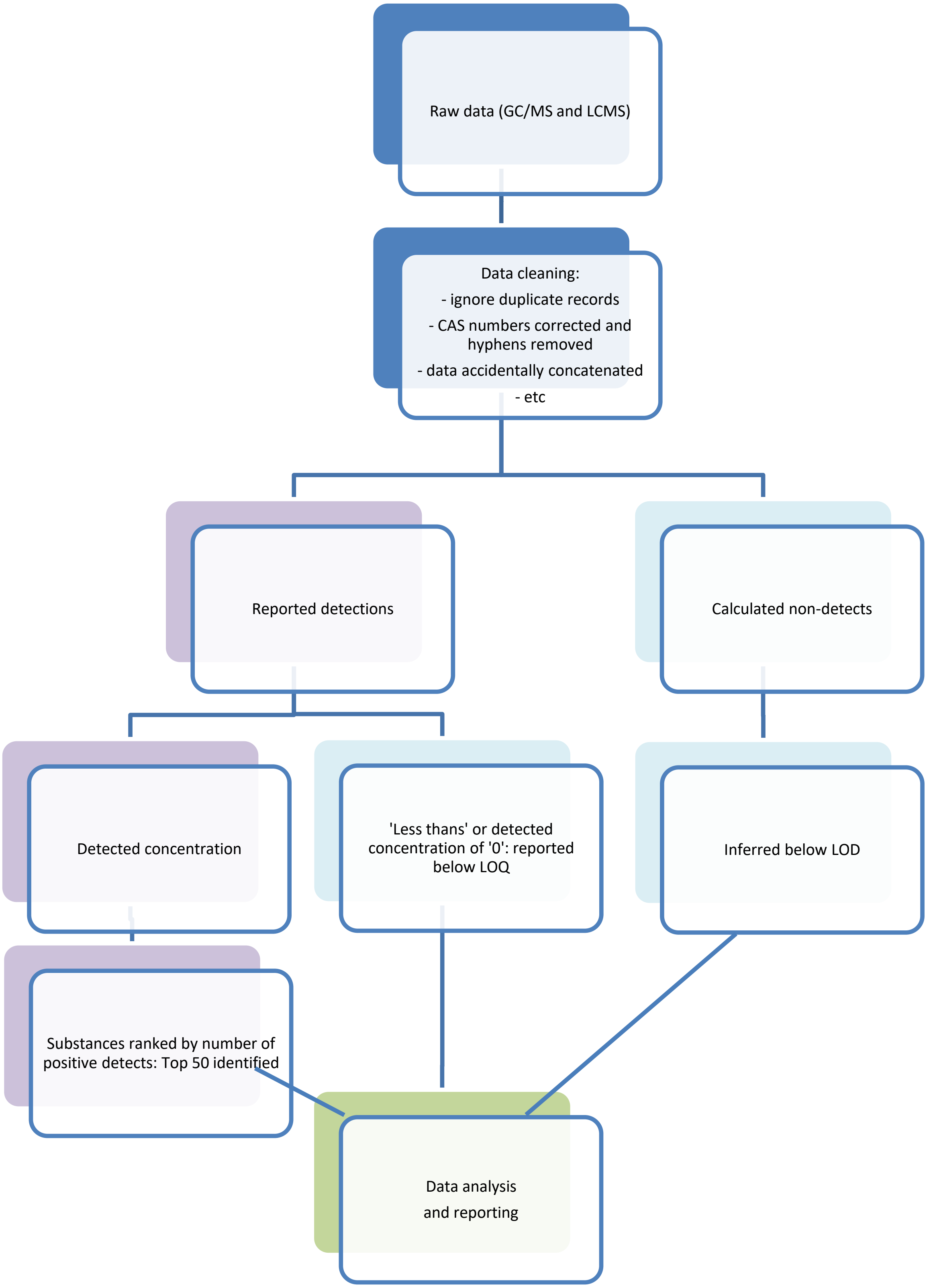

Figure 2.1. Summary workflow diagram

2.2.4 Calculating non-detects

In order to calculate the proportion of samples in which a positive detection of a compound was made, it is necessary to calculate non-detects. As these are (mostly) not reported in the Environment Agency database, they have to be calculated. Where any compound has been detected at a site on a date by the analytical method of interest (GC-MS or LC-MS), all other compounds that could be detected by that analytical method have either been detected (value in the database) or (if no value in the database) are by inference non-detects.

It is possible that samples were analysed which had no positive detects of any determinands; if this is the case there would be no record of them or the non-detects in the database.

2.3 STATISTICAL METHODS FOR DATA SETS WITH NON-DETECTS

Due to the high proportion of censored results, i.e. those reported below the method LOD, i.e. reported as "< LOD", for each compound, summary statistics were computed using the R statistical package 'NADA: Non-detects and Data Analysis for Environmental Data' (Helsel, 2012; R Core Team, 2018; Lee, 2017). Substitution methods, such as replacing non-detects with half the quantification limit or '0', are not recommended for calculation summary statistics. Two commonly used methods for estimating summary statistics (mean, median, quartiles) are maximum likelihood estimation (MLE) and robust regression on order statistics (ROS). Only where an adequate proportion of results was reported > LOD (detailed in Table 2.1), summary statistics such as the mean were computed. For large data sets ($n \geq 50$) with 50-80% of data censored the MLE is recommended, while ROS is recommended for smaller data sets or where fewer than 50% of data are censored in large data sets (Helsel, 2012). No method is recommended when censoring is higher than 80%. These recommendations were applied to the calculation of summary statistics for this report.

Table 2.1 Recommended methods for estimating summary statistics with censored data

Sample size	**Percent of data censored**		
	<50%	**50-80%**	**>80%**
n<50	ROS	ROS	censoring too high
n≥50	ROS	MLE	censoring too high

2.4 GROUPING COMPOUNDS

Compounds which have been detected by either of the analytical methods here have been classed into broad groupings to make the visualisation and description of the data more understandable. These classes are set out in Table 2.2. For many compounds, this process is straightforward with for example arable herbicides classed as pesticides, as are their transformation products (TPs) and chlorinated solvents classed as halogenated solvents.

Table 2.2 Compound use categories and short codes

Code	**Use category**	**Members**
Pest	Pesticide	Herbicides, insecticides, fungicides and their TPs
HSol	Halogenated solvent	Chlorinated solvents, trihalomethanes (THM)s
PAH	Polyaromatic hydrocarbon	Napthalene, anthracene etc
Plast	Plasticiser	Phthalates, BPA

PPCL	Pharmaceutical, Personal Care Product, Lifestyle	Pharmaceutical, including veterinary, PCPs, e.g. UV absorbers, antimicrobials and insect repellent, caffeine
Indu	Industrial	Non-halogenated solvents, other industrial and PFAS
Ster	Sterols	e.g. cholesterol, squalene – are also naturally occurring in some cases and can have high background concentrations in some situations

Pharmaceuticals are grouped together with other compounds in a broad category which is likely to enter the environment through wastewater, such as personal care products (PCPs) and caffeine. This category also includes veterinary compounds.

Assigning other compounds to a single class is difficult as they have multiple applications. UV absorbers may have both industrial and cosmetic uses, insecticides targeted at livestock or pet pests may also be classed as veterinary compounds (e.g. imidacloprid or fipronol), and industrial compounds can have a range of uses, including as plasticisers.

The use of some compounds has changed over time. Atrazine and simazine have been withdrawn in the UK for many uses since 2003 but still occur in groundwater. PFOS is another very good example: it currently has only a few restricted industrial uses, but it previously had a wide variety of uses including firefighting foams and as an impregnating agent in a number of products such as carpets, furniture, paper, textiles and leather.

This approach, while having such limitations as described above, makes the data interpretation more accessible.

3 Results from GC-MS and LC-MS datasets

3.1 TOP 50 GC-MS SUBSTANCES BY FREQUENCY OF DETECTION

3.1.1 Data description

The top 50 substances from the GC-MS dataset selected by frequency of detection are shown in Figure 3.1. A statistical summary of the data is shown in Table 3.1. Figure 3.2 shows the distribution of the results for the 50 most frequently detected substances by GC-MS using box plots. Due to the low frequency of detections, the box plots highlight the outlier values for each substance rather than the interquartile range, which for all of these substances is below the detection limit and was not computed.

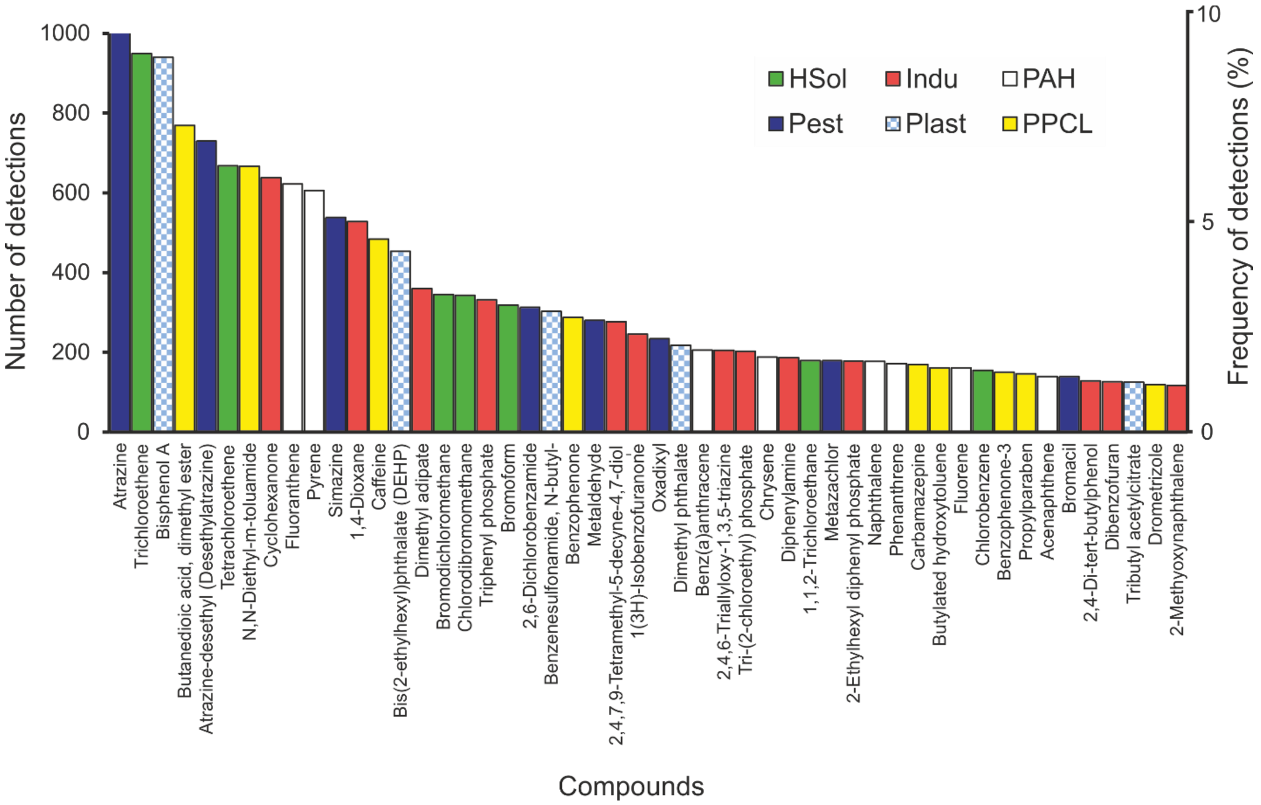

Figure 3.1. Bar chart of 50 most frequently detected substances by GC-MS screen (description of compound classes is given in Table 2.2)

Table 3.1. Summary statistics for 50 most frequently quantified substances in GC-MS screen. For all analytes the minimum concentration detected was below the LOD. The proportion of positive detections was too low to calculate a 5th percentile, median, mean or standard deviation. All concentrations are in units of µg/L.

Ranking	CAS Number	Analyte	Short name	Use code *	LOD	95th percentile concentration	Maximum concentration	Number of analyses	Number of positive detections	% analyses with positive detections
G01	1912249	Atrazine	Atrazine	Pest	0.01	0.01	0.75	11368	1069	9.40
G02	79016	Trichloroethene	TCE	HSol	0.01	0.13	184	11368	948	8.34
G03	80057	Bisphenol A	BPA	Plast	0.01	0.09	100	11368	939	8.26
G04	106650	Butanedioic acid, dimethyl ester	Dimethyl succinate	PPCL	0.01	0.02	74	11368	769	6.76
G05	6190654	Atrazine-desethyl (Desethylatrazine)	Desethyl-atrazine	Pest	0.01	0.01	1	11368	728	6.40
G06	127184	Tetrachloroethene	PCE	HSol	0.01	0.14	180	11368	668	5.88
G07	134623	N,N-Diethyl-m-toluamide	DEET	PPCL	0.01	0.01	17	11368	666	5.86
G08	108941	Cyclohexanone	Cyclohexanone	Indu	0.01	0.04	300	11368	638	5.61
G09	206440	Fluoranthene	Fluoranthene	PAH	0.01	0.01	3.4	11368	622	5.47
G10	129000	Pyrene	Pyrene	PAH	0.01	0.01	2	11368	606	5.33
G11	122349	Simazine	Simazine	Pest	0.01	0.01	0.42	11368	538	4.73
G12	123911	1,4-Dioxane	1,4-dioxane	Indu	0.01	0.01	63	11368	527	4.64
G13	58082	Caffeine	Caffeine	PPCL	0.01	0.01	1.8	11368	484	4.26
G14	117817	Bis(2-ethylhexyl)phthalate (DEHP)	DEHP	Plast	1	1	62	11368	452	3.98
G15	627930	Dimethyl adipate	Dimethyl adipate	Indu	0.01	0.01	150	11368	360	3.17
G16	75274	Bromodichloromethane	Bromodichloromethane	HSol	0.01	0.01	150	11368	344	3.03
G17	124481	Chlorodibromomethane	Chlorodibromomethane	HSol	0.01	0.01	180	11368	342	3.01
G18	115866	Triphenyl phosphate	TPPA	Indu	0.01	0.01	2	11368	331	2.91

Ranking	CAS Number	Analyte	Short name	Use code *	LOD	95th percentile concentration	Maximum concentration	Number of analyses	Number of positive detections	% analyses with positive detections
G19	75252	Bromoform	Bromoform	HSol	0.01	0.01	96	11368	318	2.80
G20	2008584	2,6-Dichlorobenzamide	BAM	Pest	0.01	0.01	70	11368	313	2.75
G21	3622842	Benzenesulfonamide, N-butyl-	BBSA	Plast	0.2	0.2	4000	11368	302	2.66
G22	119619	Benzophenone	Benzophenone	PPCL	0.01	0.01	0.8	11368	288	2.53
G23	108623	Metaldehyde	Metaldehyde	Pest	0.01	0.01	6.4	11368	280	2.46
G24	126863	2,4,7,9-Tetramethyl-5-decyne-4,7-diol	TMDD	Indu	0.03	0.03	6	11368	277	2.44
G25	87412	1(3H)-Isobenzofuranone	1(3H)-isobenzofuranone	Indu	0.01	0.01	1.2	11368	246	2.16
G26	77732093	Oxadixyl	Oxadixyl	Pest	0.01	0.01	3	11368	234	2.06
G27	131113	Dimethyl phthalate	DMP	Plast	0.01	0.01	24	11368	217	1.91
G28	56553	Benz(a)anthracene	Benz(a)anthracene	PAH	0.01	0.01	0.59	11368	206	1.81
G29	101371	2,4,6-Triallyloxy-1,3,5-triazine	TTT	Indu	0.01	0.01	62	11368	205	1.80
G30	115968	Tri-(2-chloroethyl) phosphate	Tri-(2-chloroethyl) phosphate	Indu	0.01	0.01	65	11368	202	1.78
G31	218019	Chrysene	Chrysene	PAH	0.01	0.01	0.52	11368	188	1.65
G32	122394	Diphenylamine	Diphenylamine	Pest	0.01	0.01	3	11368	187	1.64
G33	79005	1,1,2-Trichloroethane	1,1,2-trichloroethane	HSol	0.01	0.01	14	11368	179	1.57
G34	67129082	Metazachlor	Metazachlor	Pest	0.01	0.01	44	11368	179	1.57
G35	1241947	2-Ethylhexyl diphenyl phosphate	2-ethylhexyl diphenyl phosphate	Indu	0.01	0.01	1	11368	178	1.57
G36	91203	Naphthalene	Naphthalene	PAH	0.01	0.01	1.5	11368	177	1.56
G37	85018	Phenanthrene	Phenanthrene	PAH	0.01	0.01	1.2	11368	172	1.51
G38	298464	Carbamazepine	Carbamazepine	PPCL	0.01	0.01	0.26	11368	170	1.50

Ranking	CAS Number	Analyte	Short name	Use code *	LOD	95th percentile concentration	Maximum concentration	Number of analyses	Number of positive detections	% analyses with positive detections
G39	86737	Fluorene	Fluorene	PAH	0.01	0.01	2	11368	161	1.42
G40	128370	Butylated hydroxytoluene	BHT	PPCL	0.03	0.03	8.7	11368	161	1.42
G41	108907	Chlorobenzene	Chlorobenzene	HSol	0.01	0.01	1.4	11368	155	1.36
G42	131577	Benzophenone-3	Benzophenone-3	PPCL	0.01	0.01	45	11368	150	1.32
G43	94133	Propylparaben	Propyl paraben	PPCL	0.01	0.01	36	11368	146	1.28
G44	314409	Bromacil	Bromacil	Pest	0.01	0.01	3.7	11368	139	1.22
G45	83329	Acenaphthene	Acenaphthene	PAH	0.01	0.01	5	11368	139	1.22
G46	96764	2,4-Di-tert-butylphenol	2,4-DTBP	Indu	0.01	0.01	4.6	11368	128	1.13
G47	132649	Dibenzofuran	Dibenzofuran	Indu	0.01	0.01	0.61	11368	126	1.11
G48	77907	Tributyl acetylcitrate	ATBC	Plast	0.01	0.01	45	11368	125	1.10
G49	2440224	Drometrizole	Drometrizole	PPCL	0.01	0.01	18	11368	119	1.05
G50	93049	2-Methyoxynaphthalene	Nerolin	Indu	0.01	0.01	6	11368	117	1.03

* Key to use codes given in Table 2.2

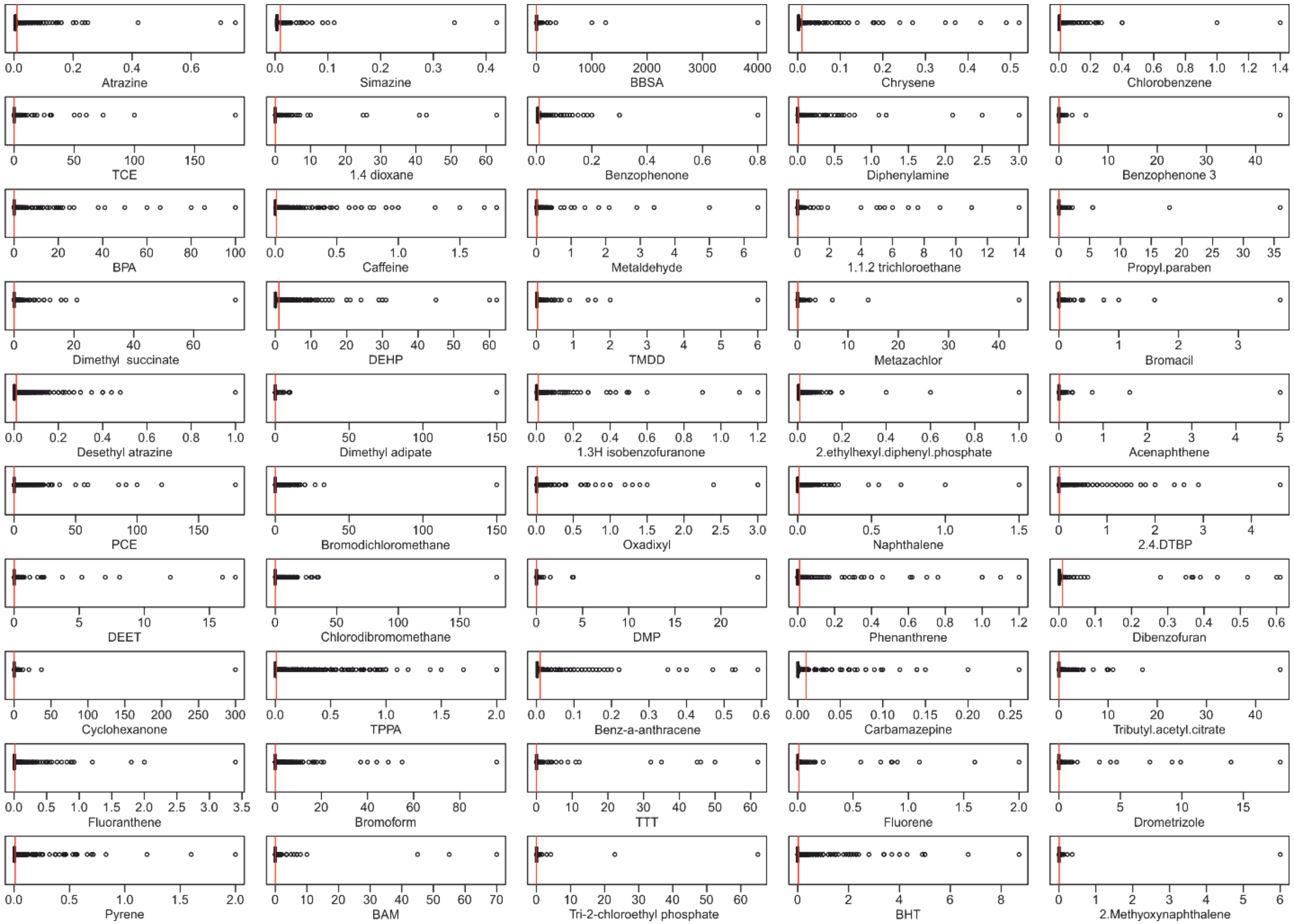

Figure 3.2. **Box plots of the 50 most frequently detected substances by GC-MS screen. x-axis shown as concentration (µg/L) for all compounds. Due to the high proportion of censored data (censored level shown as red line) summary statistics below this line are not computed.**

3.1.2 Discussion of results

Pesticides (Pest)

Eight out of the top 50 most frequently detected compounds using the GC-MS method are pesticides. The triazine herbicides remain prominent. Atrazine is the most frequently detected compound with 1069 detections corresponding to 9.4% of samples, although the concentrations are relatively low, with the 95th percentile (p95) at the LOD and a maximum concentration of 0.75 µg/L. Its TP desethyl-atrazine is also prominent, the 5th most frequently detected compound, with a slightly higher maximum concentration. Simazine is also in the top 50, the 11th most frequently detected compound, but with lower maximum concentrations. Following their withdrawal from use in the UK, in 1993 for amenity use and in 2005 for agricultural uses, concentrations of atrazine and simazine have declined considerably, but concentrations not meeting the drinking water standard still persist in a few places.

The next most frequently detected compound, 2,6-dichlorobenzamide (commonly referred to as BAM) is a TP of the herbicide dichlobenil. The p95 at the LOD, but a number of high concentrations have been measured with a maximum concentration of 70 µg/L.

Metaldehyde is a molluscicide and has been a good example of an emerging contaminant with unanticipated widespread elevated environmental concentrations found over the past decade following development of a suitable analytical method. It has been detected in 2.5% of samples with a maximum concentration of 6.4 µg/L. A ban on the outdoor use of metaldehyde is to be introduced across Great Britain from Spring 2020.

Other pesticides are oxadixyl, a fungicide used in fruit growing, diphenylamine, widely used as an industrial antioxidant and reagent and also employed in agriculture as a fungicide and antihelminthic, and the herbicides metazachlor and bromacil. These are detected in fewer than 2% of samples and have maximum concentrations in the range 3-6 µg/L except metazachlor which has a maximum concentration of 44 µg/L.

These are all compounds with a well-established track record of persistence in groundwater.

Halogenated solvents (Hsol)

Seven out of the top 50 most frequently detected compounds using the GC-MS method are halogenated solvents. Trichloroethene is the most frequently detected compound in this category, and the second overall, with 948 detections corresponding to 8.34% of samples, although the concentrations are relatively low, with a p95 of 0.13 µg/L and a maximum concentration of 184 µg/L. Tetrachloroethene and the THM bromodichloromethane are found with similar maximum concentrations but in fewer samples. Other brominated THMs detected were chlorodibromomethane and bromoform in about 2% of samples. 1,1,2-trichloroethane and chlorobenzene were also found but at lower concentrations. All compounds except trichloroethane and tetrachloroethane had censored distributions with p95 concentrations at the LOD.

Plasticisers (Plast)

Five compounds classified as plasticisers were ranked in the top 50. Of these bisphenol A was the most frequently detected, and was the third most frequent in the dataset, with 939 detections corresponding to 8.26% of samples, with a p95 of 0.09 µg/L and a maximum concentration of 100 µg/L. DEHP was detected in 4% of samples with a maximum concentration of 62 µg/L. N-butylbenzene sulphonamide was much less frequently detected (2.66%) but had a very high maximum concentration (4000 µg/L). Dimethyl phthalate and ATBC were the least frequently detected, but ATBC had a maximum detected concentration of 45 µg/L.

Industrial (Indu)

This is a diverse group of 13 compounds comprising non-chlorinated solvents, industrial intermediates and flame retardants, many of which are also used as plasticisers. All compounds in this group had censored distributions with the p95 concentration at the LOD except cyclohexanone.

NON-HALOGENATED SOLVENTS

Two compounds classed as non-halogenated solvents were detected in the top 50; 1,4-dioxane was detected in 4.6 % of samples with a maximum concentration of 63 µg/L and dimethyl adipate in 3.17% of samples but at with a higher maximum concentration of 150 µg/L. As well as a solvent 1,4-dioxane is used as a stabilizer for the transport of halogenated hydrocarbons in aluminum containers. Dimethyl adipate is a nylon precursor and it is also used as a plasticiser as well as a solvent.

INTERMEDIATES

Cyclohexanone is the most frequently detected compound in the Industrial group, found in 5.61% of samples with a maximum concentration of 300 µg/L. This has a wide range of applications and has been used in the manufacture of nylon. Other compounds were found in fewer than 2.5% of samples, TMDD, 1(3H)-isobenzofuranone ((phthalide) can also be used as a food additive), TTT, 2,4-DTBP, dibenzofuran and nerolin. They had maximum concentrations of 6 µg/L or less except TTT, which was found at 62 µg/L.

FLAME RETARDANTS

The aryl phosphate esters are mainly used as flame-retardant plasticisers in PVC and other polymers. Triphenyl phosphate is the most widely detected of these, found in 2.91% of samples with a maximum concentration of 2 µg/L. Tri-(2-chloroethyl) phosphate and 2-ethylhexyl diphenyl phosphate were found in 1.78% and 1.57% of samples with maximum concentrations of 65 µg/L and 1 µg/L respectively.

Polyaromatic hydrocarbons (PAHs)

There are 8 compounds in this category. PAHs are generally not very water soluble and are found at low concentrations. Fluoranthene and pyrene are the most soluble of these compounds and are detected in 5.47% and 5.33% of samples respectively with concentrations of 3.4 µg/L and 2 µg/L. Others are detected in fewer than 2% of samples with maximum concentrations of 2 µg/L or less except for acenaphthene which had a maximum concentration of 5 µg/L.

Pharmaceutical, personal care products, lifestyle (PPCL)

Nine of the top 50 compounds were in this category. The p95 of concentration for all of these compounds was below the LOD.

PERSONAL CARE

Compounds in this group tend to be applied to the skin. The insect repellent DEET is the most frequently detected compound in the PPCL category and the 7th overall. It was detected in 5.85% of samples with a maximum concentration of 17 µg/L. Benzophenone, benzophenone-3 and drometrizole are UV absorbers and can be used as cosmetics, such as sunscreen, and were found in 2.53% of samples at a maximum concentration of 0.8 µg/L, 1.32% of samples at a maximum concentration of 45 µg/L and 1.05% of samples at a maximum concentration of 18 µg/L respectively. The anti-microbial propyl paraben was detected in 1.28% of samples with a maximum concentration of 36 µg/L.

PHARMACEUTICALS

Relatively few pharmaceuticals are detected by the GC-MS method. Carbamazepine was detected in 1.5% of samples with a maximum concentration of 0.26 µg/L.

FOOD ADDITIVES

Butanedioic acid, dimethyl ester was the most frequently detected in this group, and the 4th most frequently overall, being detected in 6.76% of compounds with a maximum concentration of 74 µg/L. It is used as a flavouring agent but also has a wide range of industrial applications. The food antioxidant BHT was detected in 1.43% of samples with a maximum concentration of 8.7 µg/L.

LIFESTYLE

Caffeine was detected in 4.26% of samples with a maximum concentration of 1.8 µg/L.

3.2 TOP 50 GC-MS SUBSTANCES BY MAXIMUM CONCENTRATION

3.2.1 Data description

The top 50 GC-MS substances ordered by maximum concentration are shown in Figure 3.3. It is worth noting that some of these maximum concentrations (i.e. outliers) are considerably higher than the next highest concentration detected (see **Figure 3.2**), and they may represent a point source of contamination.

The top 10 highest maximum concentrations in these frequently detected compounds were for benzenesulfonamide, benzotriazole, ethylhexanoic acid, cyclohexanone, cholesterol, mercaplobenzothiazole, benzothiozole, TCE, chlorodibromomethane, and tetrachloroethene.

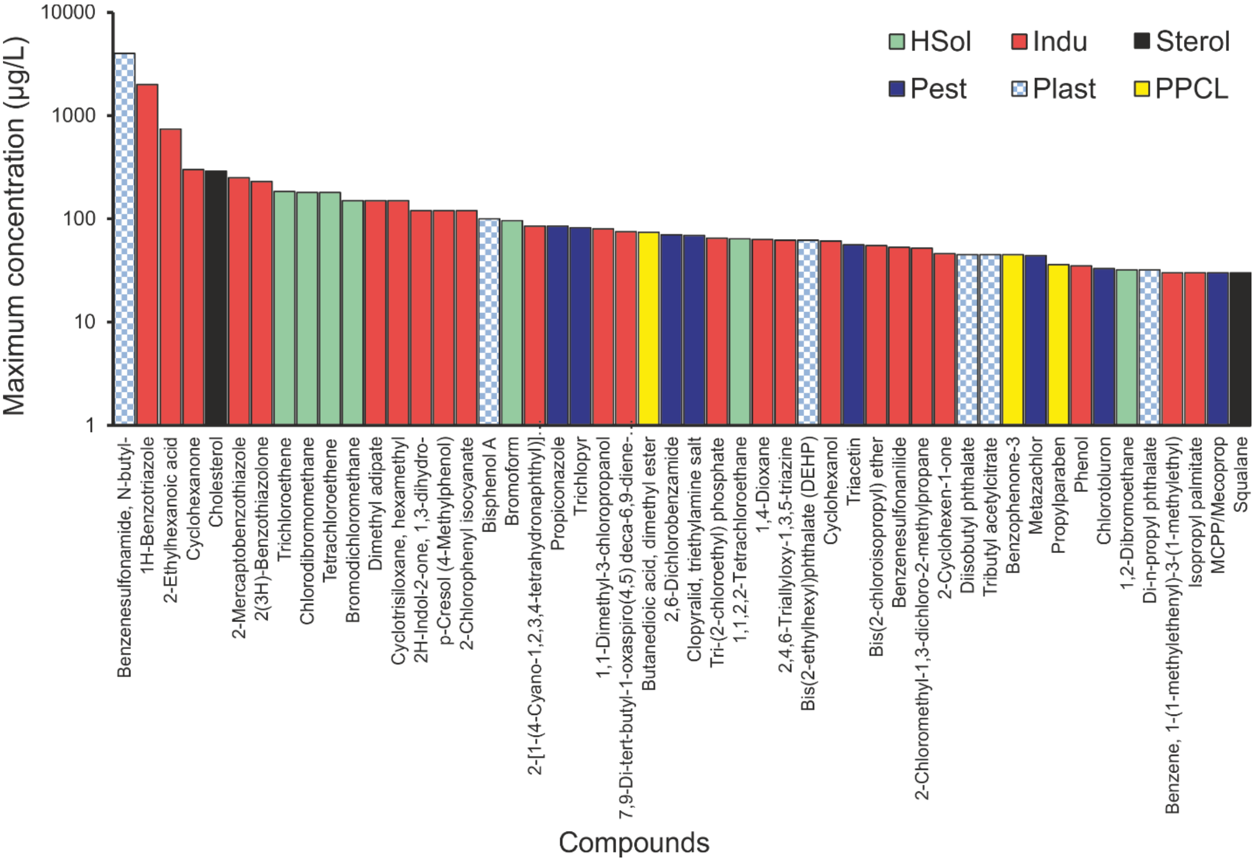

Figure 3.3. Bar chart of top 50 substances by maximum concentration by GC-MS screen

3.3 TOP 50 LC-MS SUBSTANCES BY FREQUENCY OF DETECTION

3.3.1 Data description

The top 50 substances from the LC-MS dataset selected by frequency are shown in Figure 3.4. A statistical summary of the data is shown in Table 3.2. Box plots indicating data distribution are shown in Figure 3.5

The top 18 compounds have sufficient detection data for the statistical distribution to be calculated. Many of these compounds have a median concentration considerably below the LOD. For the majority of these distributions, the p95 is at or close to the LOD. The LOD for the LC-MS method used here are much lower than the GC-MS method and this may well be the main reason why the percentage of detections is much higher.

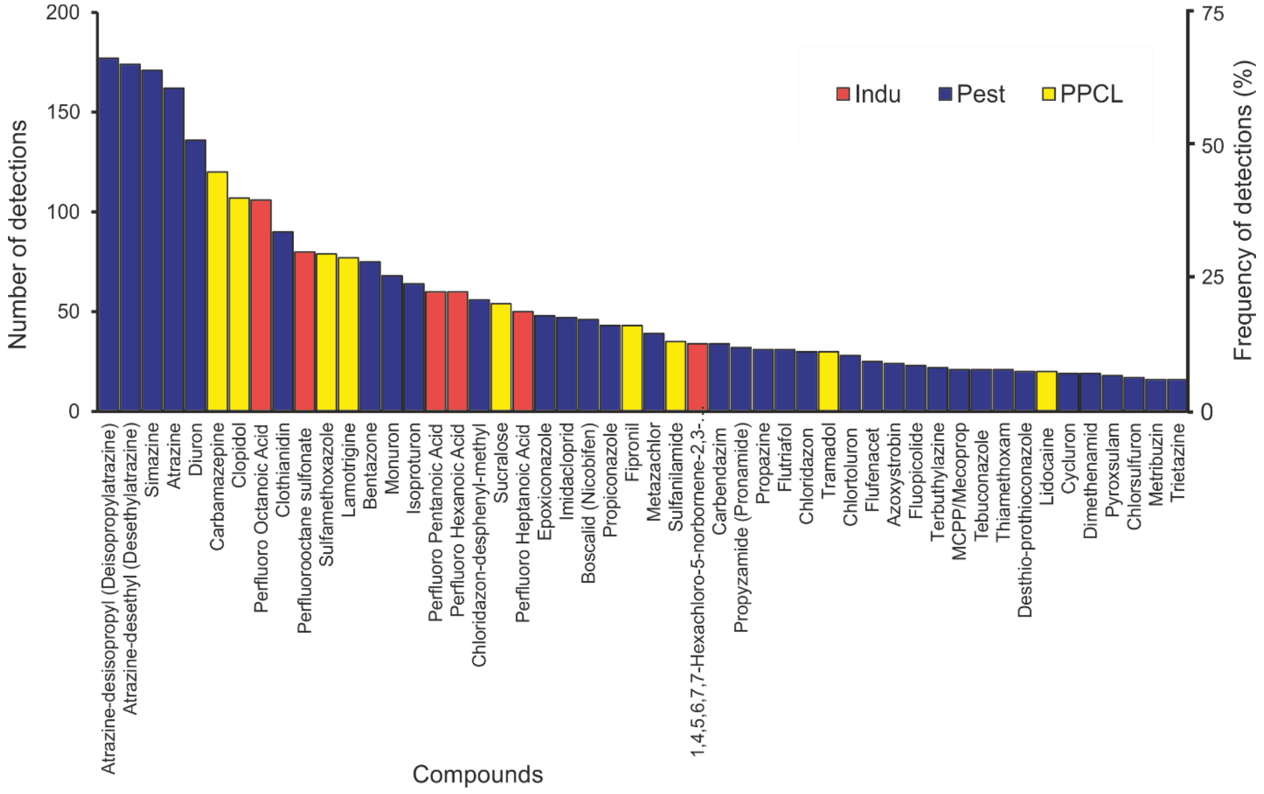

Figure 3.4. Bar chart of 50 most frequently quantified substances by LC-MS screen

Figure 3.5 shows the distribution of the results for the 50 most frequently detected substances by LC-MS using a Tukey box plot. The box plots show the interquartile range (IQR), box whiskers (values +/- 1.5 IQR) and outliers (values >1.5 IQR). In many cases the proportion of detections is too low to calculate the IQR and in these instances, the box-plots simply illustrate the outlier concentrations.

Cumulative frequency plots for the 50 most frequently detected substances by LC-MS screens are presented in Figure 3.6.

Table 3.2. Summary statistics for 50 most frequently quantified substances by LC-MS screen. For all analytes the minimum concentration detected was below the LOD. The proportion of positive detections was too low to calculate a 5th percentile value. NA = not statistically valid. Median concentration has been rounded to 6 decimal places. All concentrations are in units of µg/L.

Ranking	**CAS Number**	**Analyte**	**Short name**	**Use code ***	**LOD**	**Median concentration**	**Mean concentration**	**Standard deviation**	**95th percentile concentration**	**Maximum concentration**	**Number of analyses**	**Number of positive detections**	**% analyses with positive detections**
L1	1007289	Atrazine-desisopropyl (Deisopropylatrazine)	Desisopropyl-atrazine	Pest	0.001	0.0022	0.0064	0.007	0.02	0.05	267	176	65.92
L2	6190654	Atrazine-desethyl (Desethylatrazine)	Desethyl-atrazine	Pest	0.001	0.0021	0.018	0.03	0.07	0.3	267	172	64.42
L3	122349	Simazine	Simazine	Pest	0.001	0.001	0.004	0.005	0.02	0.03	267	170	63.67
L4	1912249	Atrazine	Atrazine	Pest	0.001	0.001	0.010	0.02	0.04	0.3	267	162	60.67
L5	330541	Diuron	Diuron	Pest	0.001	0.0005	0.0021	0.008	0.01	0.08	267	133	49.81
L6	298464	Carbamazepine	Carbamazepine	PPCL	0.001	0.0006	0.0034	0.02	0.02	0.06	267	117	43.82
L7	2971906	Clopidol	Clopidol	PPCL	0.001	0.0003	0.0045	0.067	0.02	3.5	267	106	39.70
L8	335671	Perfluorooctanoic Acid	PFOA	Indu	0.005	0.0006	0.0016	0.003	0.006	0.05	267	106	39.70
L9	210880925	Clothianidin	Clothianidin	Pest	0.001	0.0003	0.003	0.025	0.01	0.09	267	89	33.33
L10	1763231	Perfluorooctane sulfonate	PFOS	Indu	0.01	0.0002	0.003	0.03	0.01	0.4	267	80	29.96
L11	723466	Sulfamethoxazole	Sulfamethoxazole	PPCL	0.005	0.0004	0.0016	0.006	0.008	0.03	267	79	29.59
L12	84057841	Lamotrigine	Lamotrigine	PPCL	0.001	0.0003	0.001	0.003	0.006	0.04	267	76	28.46
L13	25057890	Bentazone	Bentazone	Pest	0.001	0.0001	0.024	3.8	0.03	0.9	267	75	28.09
L14	150685	Monuron	Monuron	Pest	0.001	0.0002	0.001	0.005	0.005	0.05	267	67	25.09
L15	34123596	Isoproturon	Isoproturon	Pest	0.001	0.0002	0.001	0.003	0.005	0.06	267	60	22.47
L16	2706903	Perfluoropentanoic Acid	PFPeA	Indu	0.005	0.002	0.003	0.003	0.007	0.08	267	60	22.47
L17	307244	Perfluorohexanoic Acid	PFHxA	Indu	0.005	0.001	0.002	0.003	0.005	0.13	267	60	22.47
L18	17254807	Chloridazon-desphenyl -methyl	CDM	Pest	0.001	4E-05	0.04	39.3	0.04	1.1	267	56	20.97

Ranking	**CAS Number**	**Analyte**	**Short name**	**Use code ***	**LOD**	**Median concentration**	**Mean concentration**	**Standard deviation**	**95th percentile concentration**	**Maximum concentration**	**Number of analyses**	**Number of positive detections**	**% analyses with positive detections**
L19	56038132	Sucralose	Sucralose	PPCL	0.01	NA	NA	NA	0.26	2.3	267	52	19.48
L20	375859	Perfluoroheptanoic Acid	PFHpA	Indu	0.005	NA	NA	NA	0.005	0.03	267	50	18.73
L21	133855988	Epoxiconazole	Epoxiconazole	Pest	0.004	NA	NA	NA	0.004	0.03	267	47	17.60
L22	188425856	Boscalid (Nicobifen)	Boscalid	Pest	0.005	NA	NA	NA	0.008	0.24	267	45	16.85
L23	138261413	Imidacloprid	Imidacloprid	Pest	0.001	NA	NA	NA	0.002	0.02	267	43	16.10
L24	60207901	Propiconazole	Propiconazole	Pest	0.001	NA	NA	NA	0.006	0.12	267	43	16.10
L25	120068373	Fipronil	Fipronil	Pest	0.001	NA	NA	NA	0.001	0.004	267	43	16.10
L26	67129082	Metazachlor	Metazachlor	Pest	0.001	NA	NA	NA	0.01	0.8	267	39	14.61
L27	63741	Sulfanilamide	Sulfanilamide	PPCL	0.01	NA	NA	NA	0.01	0.037	267	35	13.11
L28	115286	1,4,5,6,7,7-Hexachloro-5-norbornene-2,3-dicarboxylic acid	Chlorendic acid	Indu	0.005	NA	NA	NA	0.09	2.1	267	34	12.73
L29	10605217	Carbendazim	Carbendazim	Pest	0.01	NA	NA	NA	0.005	0.25	267	33	12.36
L30	23950585	Propyzamide (Pronamide)	Propyzamide	Pest	0.001	NA	NA	NA	0.001	0.044	267	32	11.99
L31	76674210	Flutriafol	Flutriafol	Pest	0.001	NA	NA	NA	0.01	0.1	267	31	11.61
L32	139402	Propazine	Propazine	Pest	0.001	NA	NA	NA	0.001	0.005	267	30	11.24
L33	27203925	Tramadol	Tramadol	PPCL	0.001	NA	NA	NA	0.001	0.048	267	29	10.86
L34	1698608	Chloridazon (PAC)	Chloridazon	Pest	0.001	NA	NA	NA	0.001	0.03	267	29	10.86
L35	15545489	Chlortoluron (Chlorotoluron)	Chlortoluron	Pest	0.002	NA	NA	NA	0.002	0.13	267	27	10.11
L36	142459583	Flufenacet (Fluthiamide) (BAY FOE 5043)	Flufenacet	Pest	0.001	NA	NA	NA	0.001	0.057	267	25	9.36
L37	131860338	Azoxystrobin	Azoxystrobin	Pest	0.001	NA	NA	NA	0.003	0.02	267	24	8.99
L38	5915413	Terbuthylazine	Terbuthylazine	Pest		NA	NA	NA	0.001	0.005	267	22	8.24
L39	239110157	Fluopicolide	Fluopicolide	Pest	0.001	NA	NA	NA	0.001	0.008	267	21	7.87

Ranking	CAS Number	Analyte	Short name	Use code *	LOD	Median concentration	Mean concentration	Standard deviation	95th percentile concentration	Maximum concentration	Number of analyses	Number of positive detections	% analyses with positive detections
L41	107534963	Tebuconazole (Terbuconazole)	Tebuconazole	Pest	0.001	NA	NA	NA	0.003	0.08	267	21	7.87
L40	7085190	MCPP/Mecoprop	MCPP	Pest	0.005	NA	NA	NA	0.01	0.55	267	21	7.87
L42	153719234	Thiamethoxam	Thiamethoxam	Pest	0.001	NA	NA	NA	0.001	0.003	267	20	7.49
L43	137586	Lidocaine (Diocaine)	Lidocaine	PPCL	0.001	NA	NA	NA	0.001	0.008	267	20	7.49
L44	120983644	Desthio-prothioconazole	Desthio-prothioconazole	Pest	0.001	NA	NA	NA	0.001	0.02	267	20	7.49
L45	2163691	Cycluron	Cycluron	Pest	0.001	NA	NA	NA	0.001	0.08	267	19	7.12
L46	87674688	Dimethenamid (SAN 582H)	Dimethenamid	Pest	0.001	NA	NA	NA	0.001	0.01	267	18	6.74
L47	422556089	Pyroxsulam	Pyroxsulam	Pest	0.005	NA	NA	NA	0.005	0.003	267	18	6.74
L48	64902723	Chlorsulfuron	Chlorsulfuron	Pest	0.001	NA	NA	NA	0.001	0.004	267	17	6.37
L49	21087649	Metribuzin	Metribuzin	Pest	0.002	NA	NA	NA	0.002	0.03	267	16	5.99
L50	1912261	Trietazine	Trietazine	Pest	0.005	NA	NA	NA	0.005	0.18	267	16	5.99

* Key to use codes given in Table 2.2

Figure 3.5. Box plots for the 50 most frequently detected substances by LC-MS. x-axis shown as concentration (µg/L) for all compounds. Percentiles below the red line, which shows the censored level, were estimated using regression on order statistics (ROS).

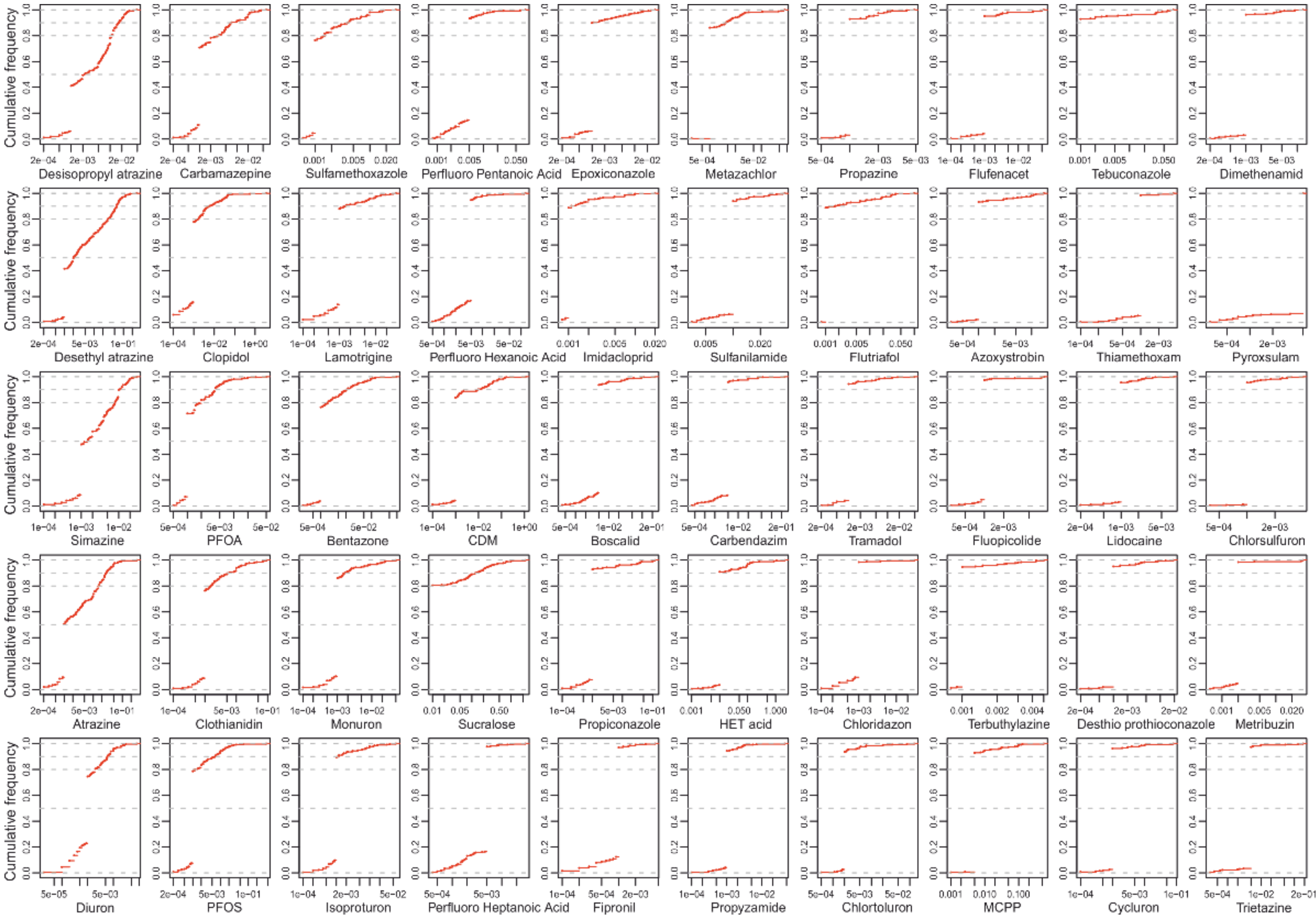

Figure 3.6. **Cumulative frequency plots for 50 most frequently detected substances by LC-MS, x-axis shown as concentration units of µg/L for all compounds**

3.3.2 Discussion of results

Pesticides (Pest)

Thirty six of the top 50 compounds most frequently detected are pesticides. The top 4 are all triazine herbicidal compounds: atrazine, the 2 main atrazine TPs and simazine. All 4 are detected in over 50% of samples. Median concentrations ranged from 0.001 to 0.002 µg/L with maximum concentrations in the ranging from 0.03 µg/L for simazine to 0.31 µg/L for atrazine.

Three ‘uron’ herbicides are in the top 15 most frequently detected pesticides: diuron in 49.8% of samples, monuron in 25.1% and isoproturon in 22.5%. Other ‘urons’ detected were chlorotoluron, cycluron and chlorsulfuron.

Other top 50 compounds were the neonicotinoid insecticide clothianidin, the herbicide bentazone and the herbicide TP chloridazon-desphenyl-methyl, all detected in more than 20% of samples. Many of the most frequently detected pesticides are no longer approved for use. The most frequently detected pesticide that is currently approved is bentazone and that was detected in 28% of samples.

Of the other pesticide compounds detected, 2 were insecticides (fipronil and imidacloprid), 9 were fungicides (epoxiconazole, propiconazole, boscalid, carbendazim, azoxystrobin, tebuconazole, fluopicolide, thiamethoxam and the TP prothioconazole-desthio) and the remaining 12 compounds were herbicides (including the parent chloridazon). All were detected in 6% of samples or more. It is interesting that the parent prothioconazole does not appear in the top 50 compounds, although it is detectable by this method. This may relate to the rapid breakdown of the parent molecule in the environment. It was introduced in 2002 as a foliar treatment for fungal diseases in cereals and is still used in the UK.

Compounds with maximum concentrations above the 0.1 µg/L drinking water limit, in descending order of concentration were chloridazon-desphenyl-methyl (1.1 µg/L), bentazone, metazachlor, 2-methyl-4-chlorophenoxyacteic acid (MCPA), atrazine, atrazine-desethyl, carbendazim, boscalid, trietazine, chlorotoluron, propiconazole and flutriafol.

Industrial compounds (Indu)

There are 6 compounds in this group, 5 of which are perfluorinated acids and esters. As might be anticipated, PFOA is the most frequently detected, in 39.7% of samples with a median concentration of 0.0006 µg/L and a maximum concentration of 0.05 µg/L, and PFOS is next, in 30% of samples with a median concentration of 0.0003 µg/L and a maximum concentration of 0.44 µg/L. The other three are the shorter chain acids, PFPeA, PFHxA and PFHpA, present in between 18.7 and 22.4% of samples with maximum concentrations of 0.08, 0.13 and 0.03 µg/L respectively.

Chlorendic acid is an industrial intermediate used in the synthesis of flame retardants and polymers. It is also a common breakdown product of several organochlorine insecticides. It was detected in 12.7% with a maximum concentration of 2.1 µg/L.

Pharmaceutical, personal care products, lifestyle (PPCL)

PHARMACEUTICALS

There are eight compounds in this group. The most widely detected compound, and 6th overall is carbamazepine, one of a number of compounds used to treat epilepsy/convulsions/bipolar disorder. This was detected in 43.8% of samples at a median concentration of 0.0006 µg/L and a maximum of 0.61 µg/L. Lamotrigine was also detected in 28.5% with a median concentration of 0.003 µg/L and a maximum of 0.036 µg/L.

Antibiotic and antibacterial compounds were detected: sulfamethoxazole in 29.6% of samples with a median concentration of 0.0004 µg/L and a maximum of 0.03 µg/L, and sulphanilamide in 13.1% with a maximum concentration of 0.037 µg/L.

The analgesics/anaesthetics tramadol and lidocaine were detected in 10.9% and 7.4% of samples respectively at maximum concentrations of 0.048 and 0.008 µg/L respectively.

The veterinary antiprotozoal substance clopidol was detected in 39.7% of samples with a median concentration of 0.0003 µg/L and a maximum concentration of 3.5 µg/L.

LIFESTYLE

The artificial sweetener sucralose was detected in 19.5% of samples with a maximum concentration of 2.3 µg/L. Sucralose has been suggested as an indicator of wastewater ingress to groundwater.

3.4 TOP 50 LC-MS SUBSTANCES BY MAXIMUM CONCENTRATION

3.4.1 Data description

The top 50 LC-MS substances ordered by maximum concentration are shown in Figure 3.3. It is worth noting that some of these maximum concentrations are considerably higher than the next highest concentration detected (see Figure 3.5), and although they may represent a highly contaminated sample.

The top 10 highest maximum concentrations were for clopidol, followed by sucralose, chlorendic acid, triallate, pentobarbital, chloridazon-desphenyl-methyl, bentazone, tridimefon, metazachlor and mecoprop, with 3 of the top 5 being PPCL compounds.

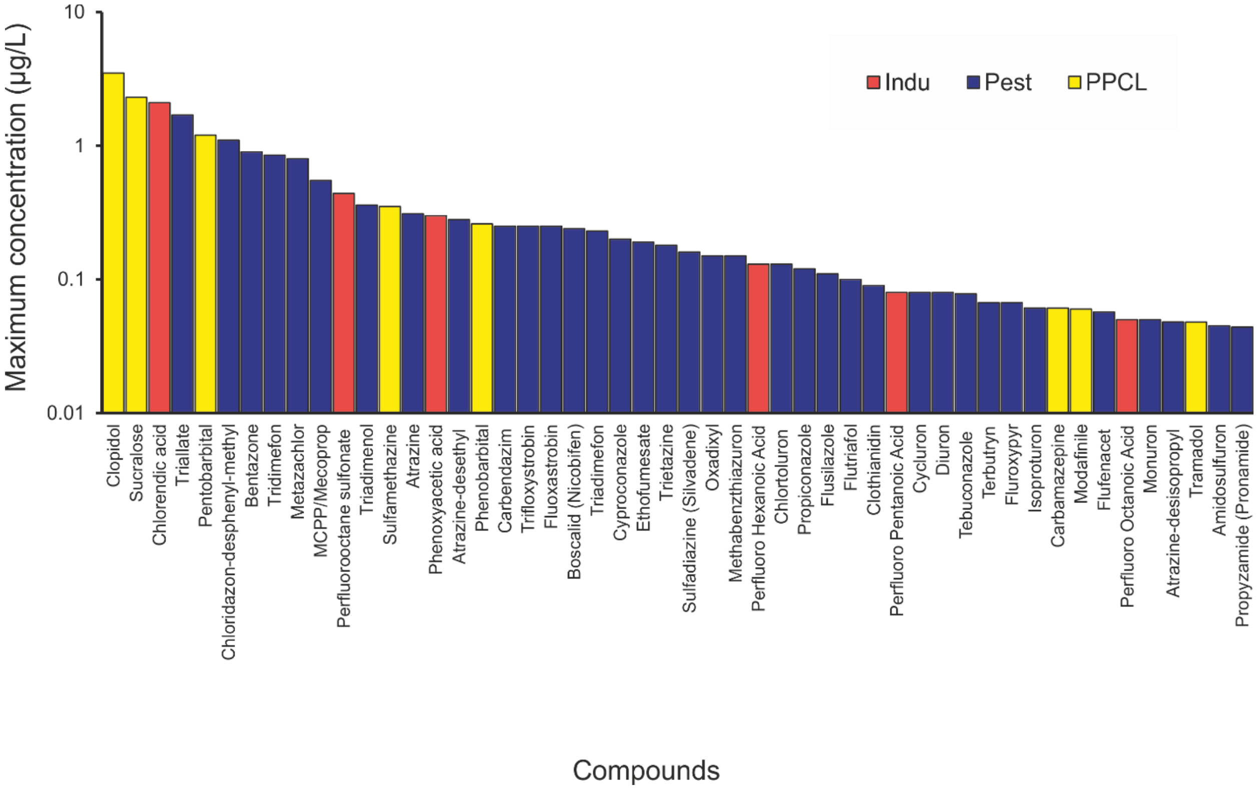

Figure 3.7. Bar chart of top 50 substances by maximum concentration by LC-MS screen

3.5 OVERLAP OF SUBSTANCES IN GC-MS-LC-MS SCREENS

Comparing the compounds listed in the Top 50 by frequency of detection and Top 50 by concentration for the GC-MS and LC-MS screens identifies 5 compounds which are detected by both methods. These compounds are listed in Table 3.3.

Table 3.3. Compounds quantified by both GC-MS and LC-MS screens, and which were ranked in the Top 50 by frequency of detection and/or concentration.

CAS Number	Analyte
122349	Simazine
298464	Carbamazepine
1912249	Atrazine
6190654	Atrazine-desethyl (Desethylatrazine)
67129082	Metazachlor

Analysis of the complete dataset indicates that the GC-MS method detected 663 substances in samples and the LC-MS detected 178 substances. Of these, 81 substances were detected by both methods: these are listed in Table 3.4.

Table 3.4. Compounds quantified by both GC-MS and LC-MS screens, in the entire BGS database

CAS Number	Analyte
50362	Cocaine
60515	dimethoate
63252	Carbaryl
72446	Methaqualone
76744	Pentobarbital
94757	2,4-D
101428	Fenuron (N,N-Dimethyl-N-phenylurea)
121755	Malathion
122349	Simazine
125406	Butabarbital (Secubarbital)
137586	Lidocaine (Diocaine)
139402	Propazine
150685	Monuron
298464	Carbamazepine
330541	Diuron
330552	Linuron
333415	Diazinon (Dimpylate)
439145	Diazepam
470906	Chlorfenvinphos
486566	Cotinine
551928	Dimetridazole
886500	Terbutryn
1007289	Atrazine-desisopropyl (Deisopropylatrazine)
1014693	Desmetryn
1689845	Bromoxynil

1698608	Chloridazon (PAC)
1912249	Atrazine
1912261	Trietazine
2303175	Triallate
2631405	Isoprocarb
2921882	Chlorpyrifos
5915413	Terbuthylazine
6190654	Atrazine-desethyl (Desethylatrazine)
7287196	Prometryn
15299997	Napropamide
15545489	Chlorotoluron
15687271	Ibuprofen
16118493	Carbetamide
18691979	Methabenzthiazuron
19666309	Oxadiazon
21087649	Metribuzin
21725462	Cyanazine (Fortrol)
23103982	Pirimicarb
23950585	Propyzamide (Pronamide)
25057890	Bentazone
26225796	Ethofumesate
28721075	Oxcarazepine
29232937	Pirimiphos-methyl (Pirimifos-methyl)
34123596	Isoproturon
40487421	Pendimethalin (Penoxalin)
43121433	Triadimefon
51235042	Hexazinone
53112280	Pyrimethanil
55219653	Triadimenol
55335063	Trichlopyr
57837191	Metalaxyl
60142963	Gabapentin
60168889	Fenarimol
60207901	Propiconazole
66246886	Penconazole
66332965	Flutolanil
67129082	Metazachlor
67564914	Fenpropimorph (Ro 14-3169)
67747095	Prochloraz
76674210	Flutriafol
77732093	Oxadixyl
85509199	Flusilazole
87674688	Dimethenamid (SAN 582H)
107534963	Tebuconazole (Terbuconazole)
110488705	Dimethomorph
120068373	Fipronil
121552612	Cyprodinil

123312890	Pymetrozin
131860338	Azoxystrobin
133855988	Epoxiconazole
142459583	Flufenacet (Fluthiamide) (BAY FOE 5043)
153719234	Thiamethoxam
183675823	Penthiopyrad
188425856	Boscalid (Nicobifen)
239110157	Fluopicolide
361377299	Fluoxastrobin

3.6 SPATIAL PLOTS OF OCCURRENCE OF SELECTED SUBSTANCES

This section presents a series of spatial plots of key substances. These were selected on the basis of frequency of detection and/or being classed as PPCL, a large group of substances of potential emerging concern which is receiving growing attention in Europe. Concentrations (maximum per site) are shown as proportional symbols. Results are plotted on a background of a simplified 1:625,000 scale geological map as requested by the EA: the legend is provided in Figure 3.8.

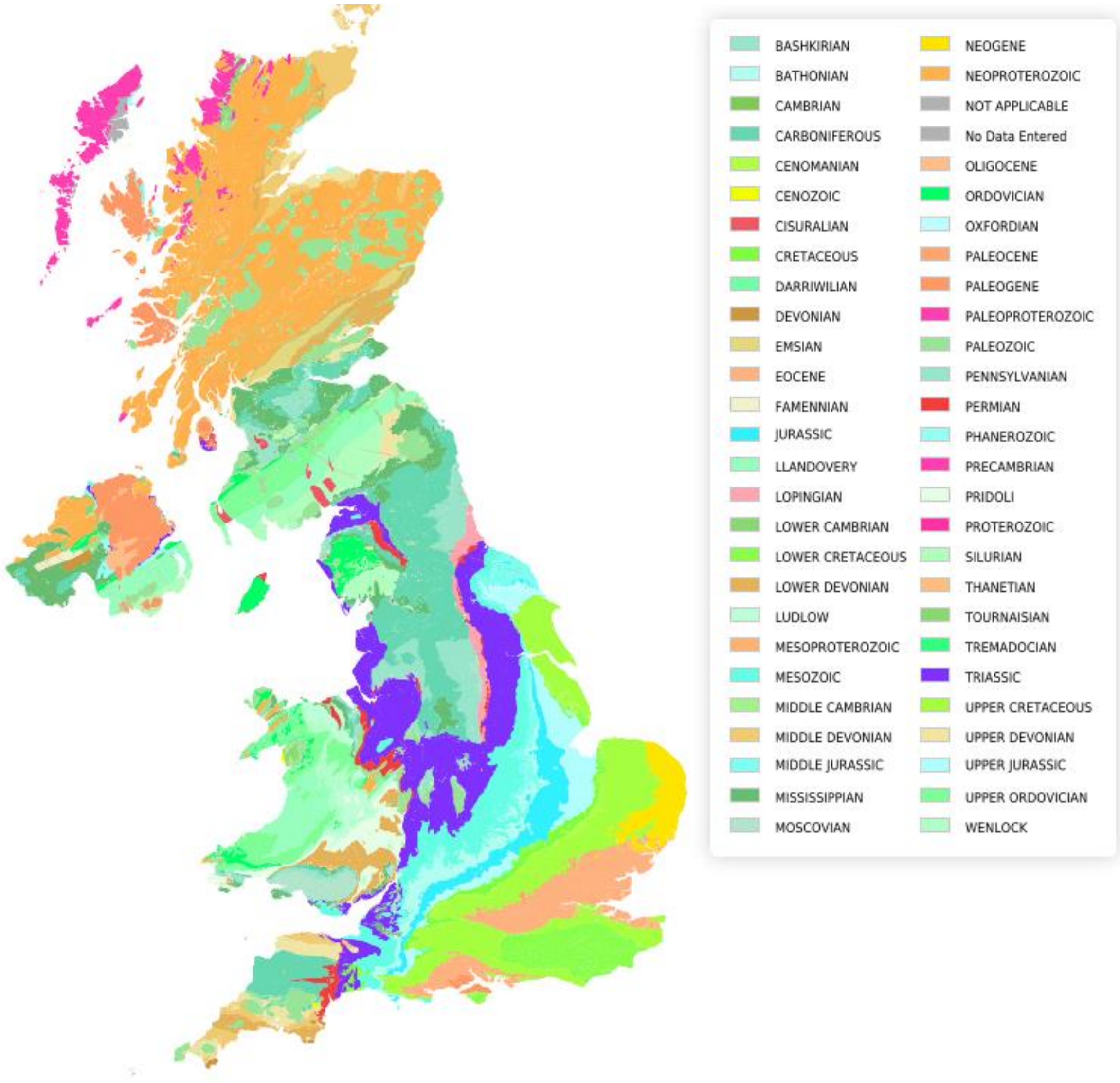

Figure 3.8. Geological map background (1:625 scale bedrock geology – UK onshore bedrock age) with legend.

3.6.1 GC-MS

Atrazine remains the most frequently detected compound by GC-MS. Since the database contains data collected throughout the period that this method has been used, it may give a misleading impression of current conditions. A spatial plot of these data (Figure 3.9) shows that atrazine is predominantly detected at concentrations of >0.1 µg/L in the principal aquifers of the Chalk and the Permo-Triassic sandstone. This may reflect historical usage and particularly for the Chalk the travel time from the surface through the unsaturated zone to the water table and the slow rate of flushing of these aquifers.

Historically atrazine was used for weed control, both in agriculture and for amenity use until 1992 when it was withdrawn from non-agricultural uses in the UK. There was concern that amenity use potentially allowed pesticide to enter the subsurface via soakaways, bypassing the soil. Limited agricultural uses were permitted until an EU-wide ban for all uses followed in 2003. The elevated concentrations seen in this dataset demonstrate that a precautionary approach is needed to protect groundwater from pesticides as degradation rates in the subsurface are typically very slow.

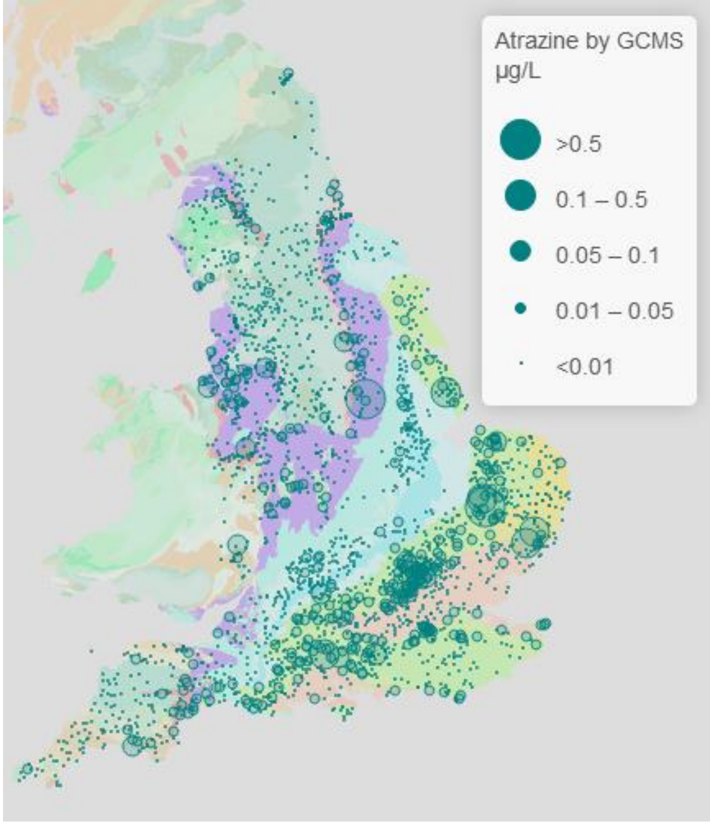

Figure 3.9. **Spatial plot of atrazine concentrations by GC-MS screen (µg/L)**

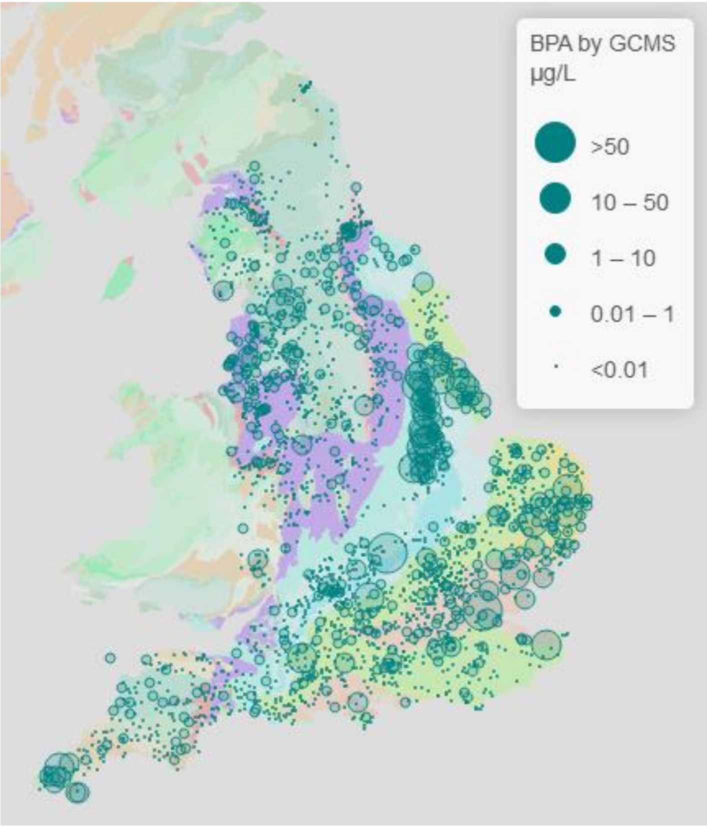

Figure 3.10. **Spatial plot of BPA concentrations by GC-MS screen (µg/L)**

BPA is the most frequently detected plasticiser in the dataset. The spatial plot (Figure 3.10) shows it to be widely detected across England. There are areas of concentrations >1 µg/L in the urban areas of Greater London and the Thames Estuary, Birmingham, Liverpool and Hull areas and in the Jurassic limestones of Lincolnshire and perhaps surprisingly in the far southwest.

There are likely to be multiple sources of BPA in the environment, including wastewater, septic tanks and landfills. It is also a common component of many plastic items and care is needed to exclude these from sampling equipment. Plasticisers can be leached into groundwater from plastic well casing and pipework associated with groundwater sampling and this could explain BPA detections at some sites rather than BPA occurrence in the aquifer.

DEET is the second most frequently detected PPCL in the dataset. Figure 3.11 shows higher concentrations to be distributed with areas of central southern England, the north Yorkshire coast and the Manchester-Liverpool area with groups of values over 0.1 µg/L. The Lincolnshire Limestone and the south east of England also show scattered higher concentrations.

When used as an insect repellent, DEET is topically applied and may therefore be found in the wastewater stream (Aronson et al., 2012). DEET can be readily absorbed into the body of plastic objects. The spatial coherence of DEET observations in some regions suggests that some detections may be due to contamination from samplers, but this has not been verified.

Butanedioic acid, dimethyl ester (dimethyl succinate) is detected widely across England, with surprisingly few detections in the Chalk of south-east England, the Carboniferous and Devon and Cornwall (Figure 3.12).

Caffeine is also widely detected in groundwater across England with pronounced clusters of detections in the London area, Cornwall and North Yorkshire (Figure 3.13).

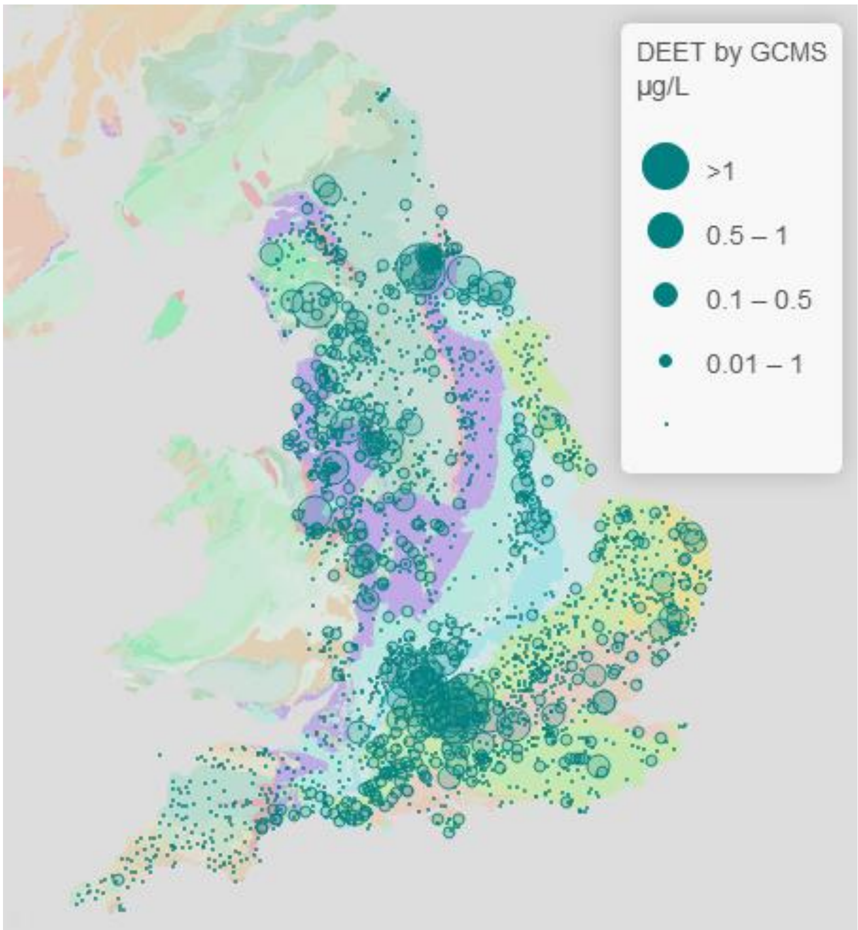

Figure 3.11. Spatial plot of DEET concentrations by GC-MS screen (µg/L)

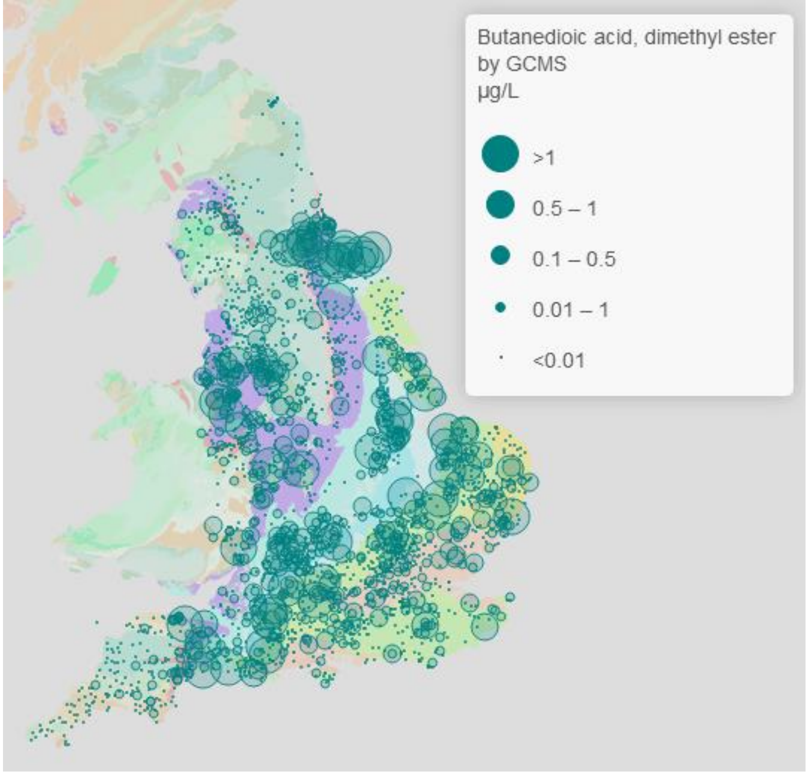

Figure 3.12. **Spatial plot of butanedioic acid, dimethyl ester (dimethyl succinate) concentrations by GC-MS screen (µg/L)**

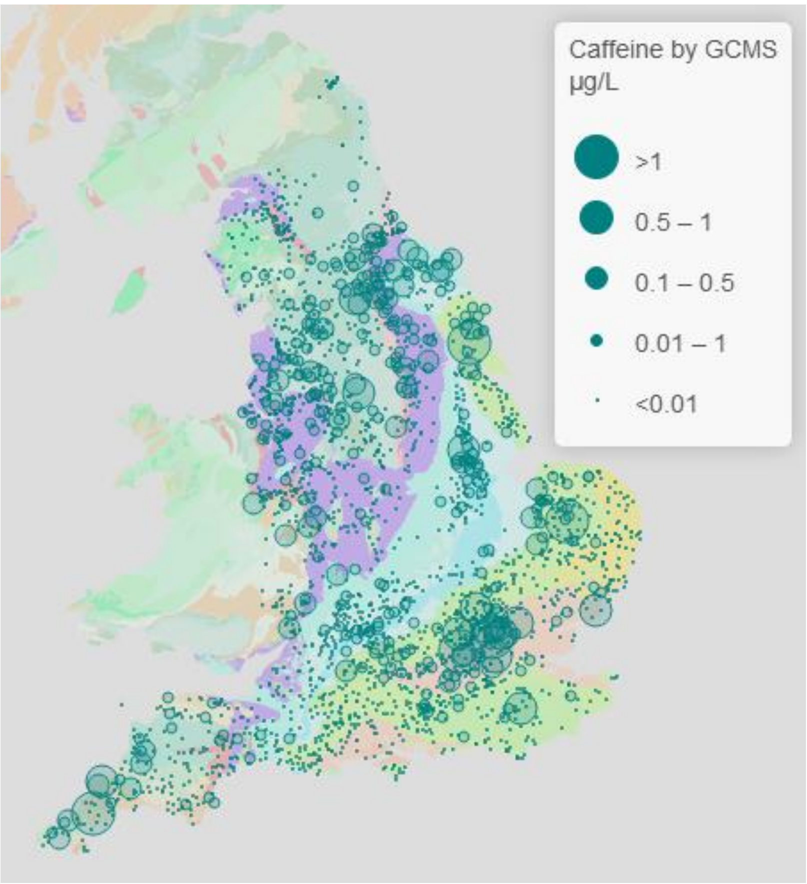

Figure 3.13. **Spatial plot of caffeine concentrations by GC-MS screen (µg/L)**

3.6.2 LC-MS

There are considerably fewer LC-MS data and these are confined to selected regions of the EA. Carbamazepine is the most frequently detected PPCL in the LC-MS database. The spatial plot (Figure 3.14) shows sampling to be mainly restricted to the central and southern areas of England, with some sampling in the northeast. Carbamazepine is detected in the London area, in the Chalk of the southeast and in the Permo-Triassic sandstone. There is insufficient data to comment on controls on spatial distribution.

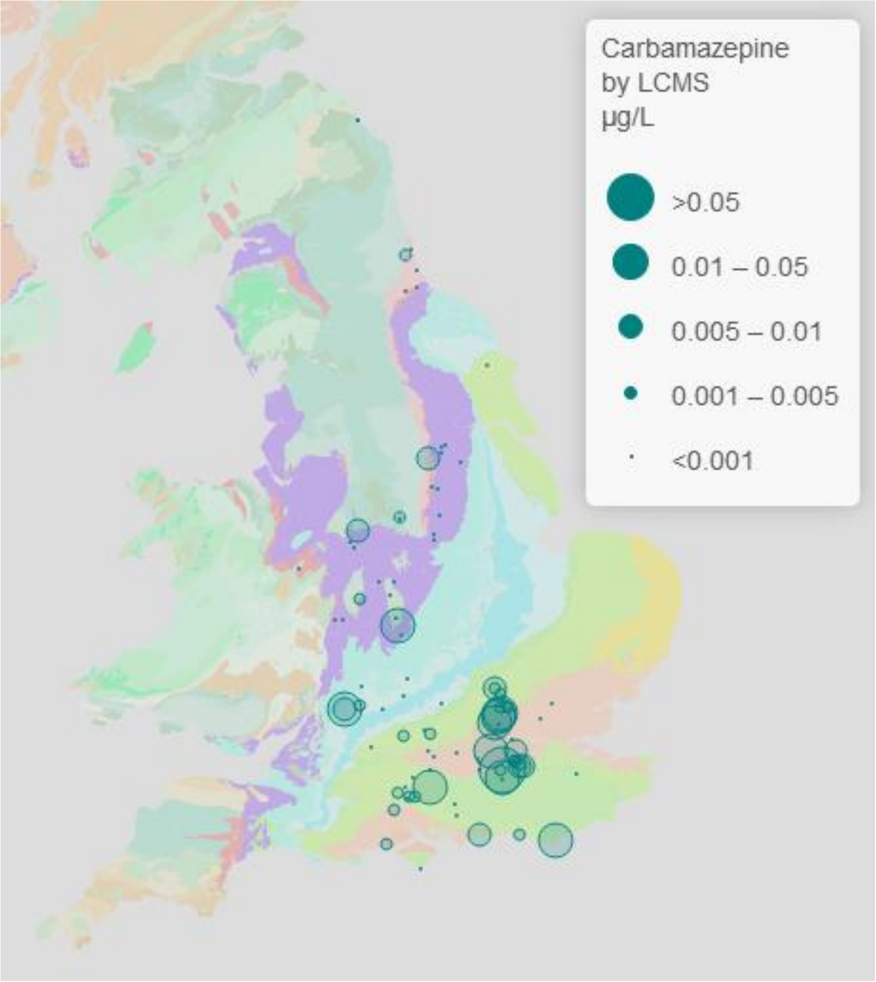

Figure 3.14. Spatial plot of carbamazepine concentrations by LC-MS screen (µg/L)

Detections of clothianidin were found in Gloucestershire and Oxfordshire, in London and in Sussex/Hampshire (Figure 3.15). Presumably, this is associated with the distribution of the target insect pests, but there are too few datapoints to allow comment on spatial distribution.

PFOS and PFOA were mainly detected in the London area, some of which are possibly associated with the Buncefield fire in 2005 and the extensive use of foams to supress the fire (Figure 3.16 and Figure 3.17). Other localised detections include in Hampshire, two sites near the coast in north east England, and a site in Birmingham. PFOS and PFOA are also degradation products of other precursor substances not reported in the LC-MS target screening method.

Clopidol was detected in µg/L concentrations at only a small number of sites, possibly associated with livestock farming and the veterinary use of this substance to treat Coccidia parasites. A high proportion of detections at low concentrations give rise to its prominence in Figure 3.18, but initial results do not indicate a wide distribution in groundwater at µg/L concentrations, however the spatial sampling is limited.

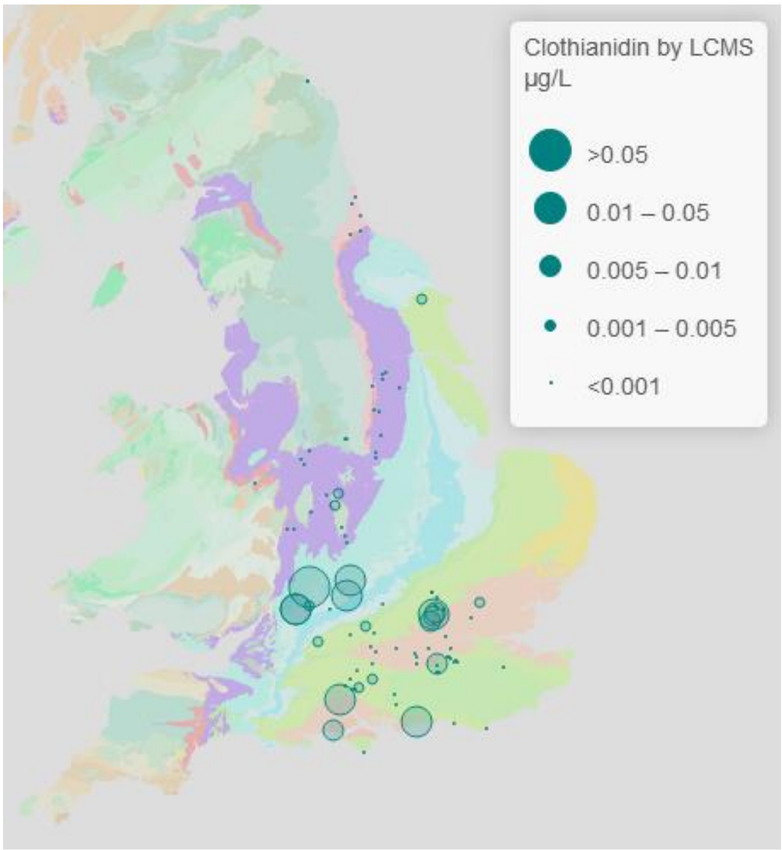

Figure 3.15. Spatial plot of clothianidin concentrations by LC-MS screen (µg/L)

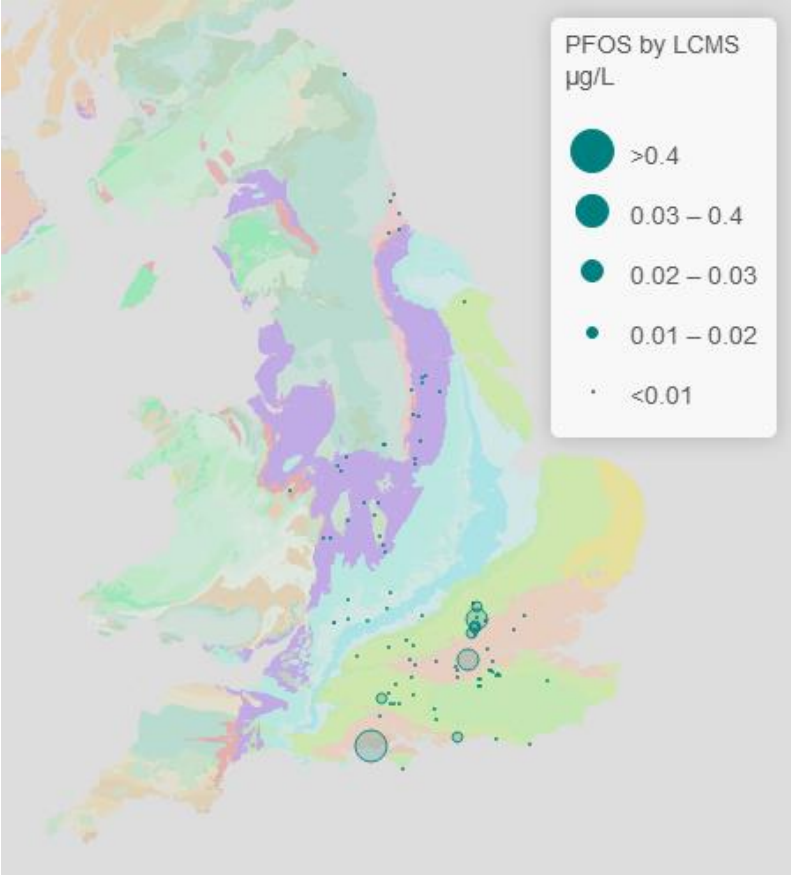

Figure 3.16. Spatial plot of PFOS concentrations by LC-MS screen (µg/L)

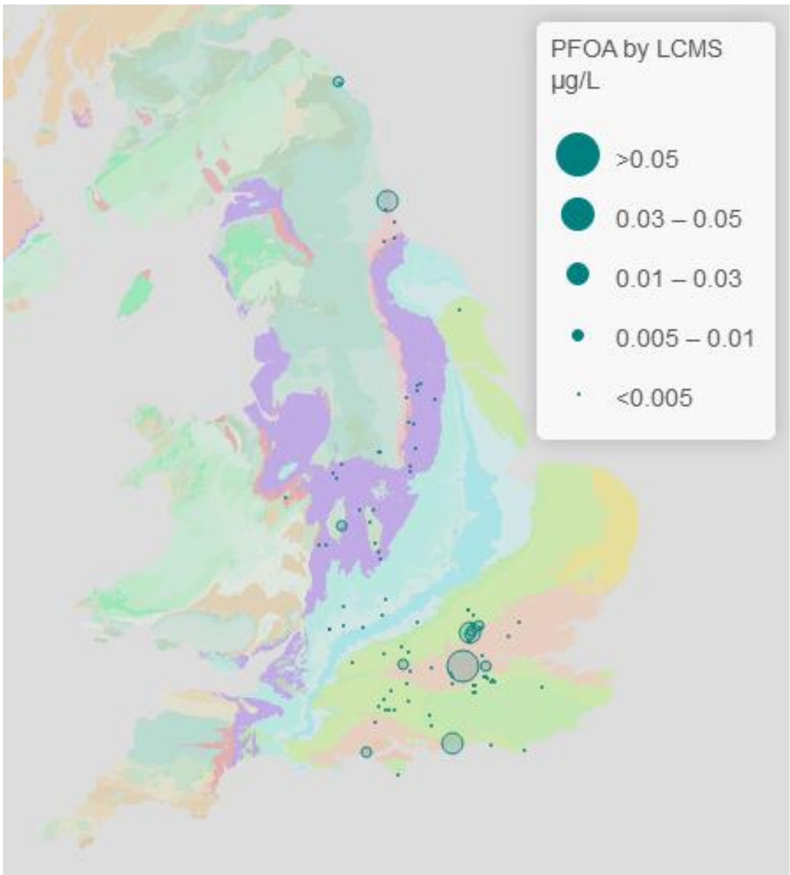

Figure 3.17. **Spatial plot of PFOA concentrations by LC-MS screen (µg/L)**

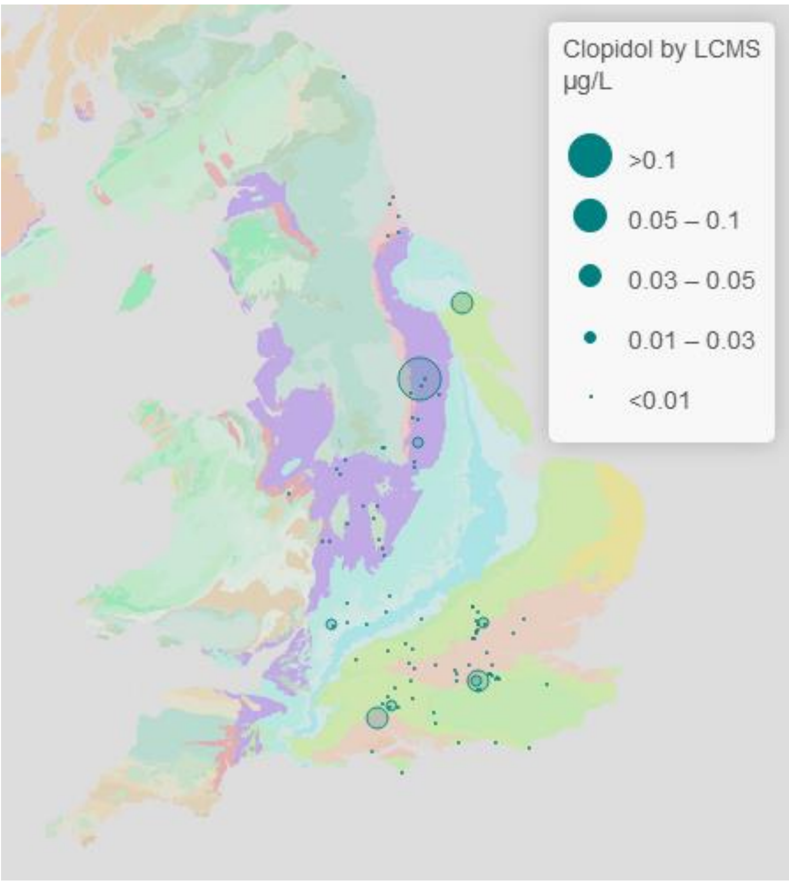

Figure 3.18. **Spatial plot of clopidol concentrations by LC-MS screen (µg/L)**

4 Emerging substances in UK groundwater

4.1 KEY SUBSTANCES WITH HIGH FREQUENCY OF DETECTION

Table 4.1 shows the ten most frequently detected substances by the GC-MS method and summary details of their regulation. Six are pesticides, or their TPs, or halogenated solvents and are covered by the Drinking Water Directive (DWD 98/83/EC). Four of these are hazardous or priority hazardous substances under by the Priority Substances Directive (2008/105/EC). Two of these also appear in Annex XIV of the REACH Regulations. None are on the surface water watch list (SWWL), which is linked to the Water Framework Directive (2000/60/EC and later amended by 2008/32/EC).

Table 4.1. Regulation of GC-MS frequently detected substances

Substance	**Type**	**Use**	**Regulation[a&b]**			
			DWD[a]	**Limit (µg/L)**	**Other**	**Status**
Atrazine	Pesticide	Herbicide	Y	0.1 (0.5 total)	PPP[b] PSD[a]	Withdrawn Hazardous substance
TCE	Halogenated solvent	Degreaser and feedstock for CFCs	Y	10 (PCE+TCE)	PSD[a] REACH [b]Annex XIV	Equivalent to Priority substance SVHC
BPA	Plasticiser	Polycarbonates and epoxy coatings	N		Food contact REACH [b]	Food packaging for infants ECHA candidate
Dimethyl succinate	PPCL	Flavouring fragrance plus industrial	N			
Desethyl-atrazine	Pesticide	Herbicide TP	Y	0.1(0.5 total)		Parent withdrawn
PCE	Halogenated solvent	Degreaser, dry cleaning	Y	10 (PCE+TCE)	PSD[a] REACH [b]Annex XIV	Equivalent to Priority substance SVHC
DEET	PPCL	Insect repellent	N		Biocide regs[b]	
Cyclo-hexanone	Industrial	Nylon precursor and many other uses	N			
Fluoranthene	PAH	Waste product	Y		PSD[a]	Priority substance
Pyrene	PAH	Waste product	Y		SVHC[b]	

DWD - Drinking Water Directive, PPP- Plant Protection Products regulation, PSD - Priority Substances Directive, SVHC – substance of very high concern (REACH Regulations). [a]end-of-pipe regulation and [b]Source regulation.

Table 4.2 shows the ten most frequently detected substances by the LC-MS method and summary details of their regulation. Six are pesticides, or their TPs, and covered by the Drinking Water Directive; four are common to Table 4.1 Three of these are hazardous or priority hazardous substances under by the Priority Substance Directive. Two are industrial/flame retardants which appear in Annex XVII of the REACH Regulations. One of the pesticides is on the SWWL.

Table 4.2. Regulation of LC-MS frequently detected substances

Substance	**Type**	**Use**	**Regulation[a&b]**			
			DWD[a]	**Limit (µg/L)**	**Other**	**Status**
Deisopropyl-atrazine	Pesticide	Herbicide TP	Y	0.1(0.5 total)		Parent withdrawn
Desethyl-atrazine	Pesticide	Herbicide TP	Y	0.1(0.5 total)		Parent withdrawn
Simazine	Pesticide	Herbicide	Y	0.1 (0.5 total)	PPP[b] PSD	Withdrawn Hazardous substance
Atrazine	Pesticide	Herbicide	Y	0.1 (0.5 total)	PPP[b] PSD[a]	Withdrawn Hazardous substance
Diuron	Pesticide	Herbicide	Y	0.1 (0.5 total)	PPP[b] PSD[a]	Withdrawn Hazardous substance
Carbamazepine	Pharmaceutical	Epilepsy/bipolar disorder	N			
Clopidol	Pharmaceutical	Veterinary	N			
PFOA	Perfluorinated organic	Industrial	N		REACH[b] Annex XVII	Restricted in consumer products
Clothianidin	Pesticide	Neonicotinoid	Y	0.1(0.5 total)	SWWL[a]	Monitored
PFOS	Perfluorinated organic	Industrial	N		PSD[a] REACH[b] Annex XVII	Priority substance Restricted

DWD - Drinking Water Directive, PPP- Plant Protection Products regulatioin, PSD - Priority Substances Directive, SWWL – surface water watch list. [a]end-of-pipe regulation and [b]Source regulation.

In some cases a substance can belong to more than one regulatory regime, these are summarised by key substances types in Table 4.3

Table 4.3. Current EU chemical substance source regulations

Chemical Substance Type	**European Legislative Body (Regulation)**
Industrial & consumer chemicals	ECHA (No. 1907/2006)
Human pharmaceuticals	EMA, EMEA/CHMP/SWP/4447/0
Veterinary medicines	EMA
Plant protection products	EFSA (EC 1107/2009)
Biocides	ECHA (EU. 528/2012)

ECHA – European Chemicals Agency, EMA-European Medicines Agency, EFSA – European Food Safety Authority

4.2 COMPARISON WITH PREVIOUS STUDIES

Most of the GC-MS data is common to this study and previous BGS studies reported in 2012 and 2016 which used Environment Agency monitoring data, but the current study differs in several respects:

- It contains more recent data up to 2018
- It has been restricted to GC-MS targeted screening data only, whereas the other studies also included some data provided by other analytical methods, e.g. SVOCs.
- The GC-MS method is continuously updated with new compounds being introduced and identification algorithms being improved to reduce false positives.

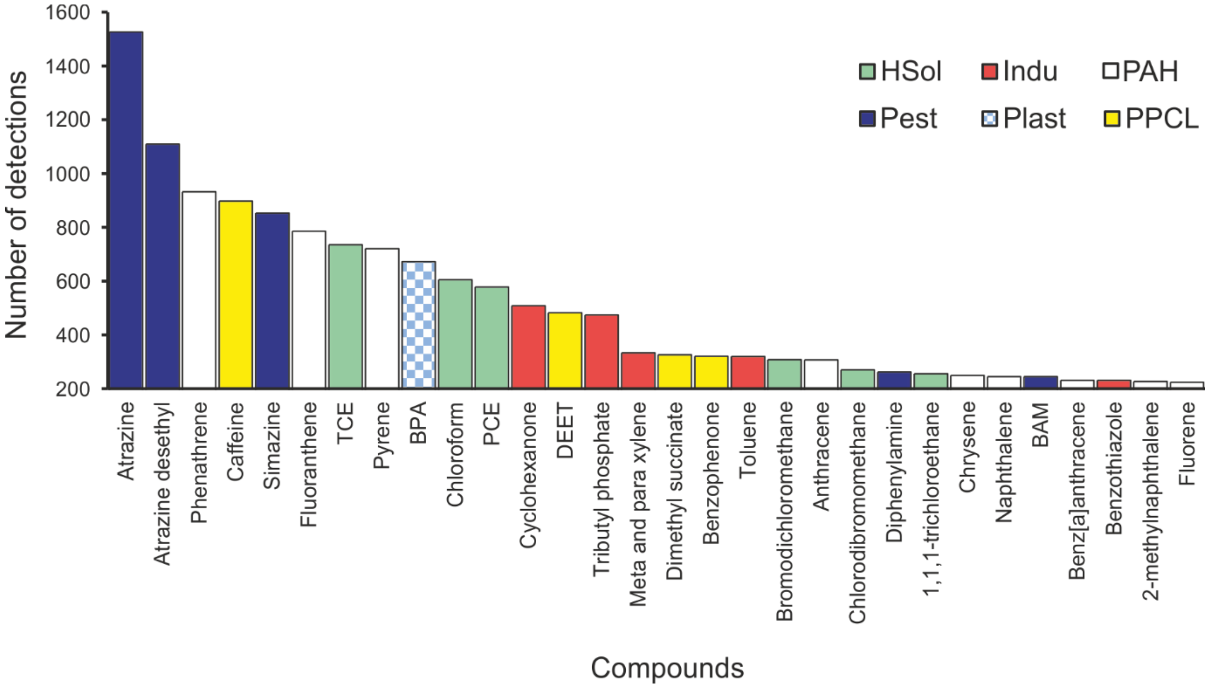

Figure 4.1. Top 30 most frequently detected compounds from 2016 assessment

Figure 4.1 shows frequency data from the 2016 study (Manamsa et al., 2016). There are fewer detections overall in the current study as results from methods other than GC-MS have been excluded. Similar compounds remain prominent in the current study in most frequent positions:

- The pesticide atrazine remains the most frequently detected compound but its desethyl TP is less prominent in this dataset
- The halogenated solvents TCE and PCE are found at higher relative frequencies as are the plasticisers BPA and DEET, and the industrial compounds cyclohexanone, dimethyl succinate and dimethyl adipate
- Caffeine has become less prominent as have some PAHs.

Figure 4.2 shows maximum concentration data from the 2016 study. Compounds in Figure 4.2 do not compare very well with the current study (Figure 3.3). This reflects the exclusion of data from non-GC-MS screening methods in this review and also that these maximum concentrations may be random outliers and do not reflect typical concentrations.

The halogenated solvents are less prominent in the current study than in Figure 4.2 and particularly reflect the exclusion of solvent data from non-GC-MS methods. Plasticisers remain prominent and BBSA is the most frequently detected compound in the current study. Of the PPCL compounds, dimethyl succinate did not appear in the top 30 in 2016.

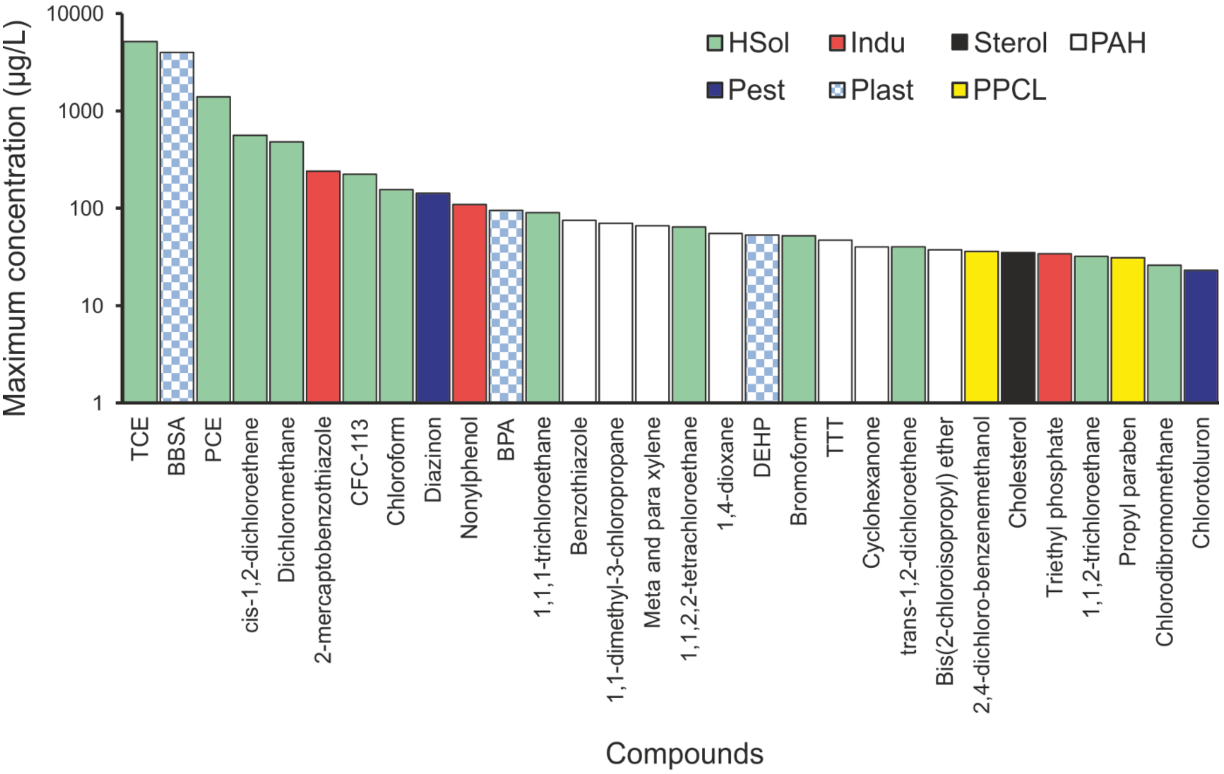

Figure 4.2. Top 30 maximum concentrations from 2016 assessment

4.3 IMPLICATIONS FOR USING QUANTITATIVE ANALYTICAL SUITES

4.3.1 Compounds detected

Many of the most frequently detected compounds in the GC-MS results would not be detected by the dedicated suites currently used by the Environment Agency. These dedicated suites are shown in Table 4.4.

Table 4.4. Environment Agency quantitative suites

Suite code	Suite name	Typical member	LOD (µg/L)
GWQM01	ONP pesticides	Atrazine & TPs, diazinon	0.001-0.02
GWQM02	ONC pesticides	Trichlorobenzene, diclobenil, PCBs, aldrin	0.001-0.02
GWQM03	Acid herbicides	Bentazone, clopyralid, mecaprop	0.005-0.04
GWQM04	Urons/urocarbs	Azoxystrobin, carbendazim, isoproturon	0.005-0.1
GWQM05	Phenols	Chlorophenols	0.002
GWQM06	VOCs	Halogenated solvents, BTEX	0.01-0.5
GWQM07	PAH	Anthracene, chrysene, fluoranthene	0.01
GWQM08	Pyrethroids	Cypermethrin	0.00001-0.0001
GWQM09	Discretionary	Chlormequat, fluazaflop-butyl	0.01-0.2
	Special-site-by-site	Glyphosate, AMPA, metaldehyde	0.01-0.1
	PFOS/PFOA		0.005-0.1

Table 4.5 indicates that 60% (30/50) of the top 50 compounds found by the GC-MS method do not appear in the standard suites. These are predominantly industrial, plasticisers and PPCL compounds with a small number of pesticides and pesticide TPs.

Table 4.5. Compounds detected by GC-MS screen not present in standard suites

Ranking	CAS Number	Analyte	Short name	Use code *
G03	80057	Bisphenol A	BPA	Plast
G04	106650	Butanedioic acid, dimethyl ester	Dimethyl succinate	PPCL
G07	134623	N,N-Diethyl-m-toluamide	DEET	PPCL
G08	108941	Cyclohexanone	Cyclohexanone	Indu
G12	123911	1,4-Dioxane	1,4-dioxane	Indu
G13	58082	Caffeine	Caffeine	PPCL
G14	117817	Bis(2-ethylhexyl)phthalate (DEHP)	DEHP	Plast
G15	627930	Dimethyl adipate	Dimethyl adipate	Indu
G18	115866	Triphenyl phosphate	TPPA	Indu
G20	2008584	2,6-Dichlorobenzamide	BAM	Pest
G21	3622842	Benzenesulfonamide, N-butyl-	BBSA	Plast
G22	119619	Benzophenone	Benzophenone	PPCL

Ranking	CAS Number	Analyte	Short name	Use code *
G24	126863	2,4,7,9-Tetramethyl-5-decyne-4,7-diol	TMDD	Indu
G25	87412	1(3H)-Isobenzofuranone	1(3H)-isobenzofuranone	Indu
G26	77732093	Oxadixyl	Oxadixyl	Pest
G27	131113	Dimethyl phthalate	DMP	Plast
G29	101371	2,4,6-Triallyloxy-1,3,5-triazine	TTT	Indu
G30	115968	Tri-(2-chloroethyl) phosphate	Tri-(2-chloroethyl) phosphate	Indu
G32	122394	Diphenylamine	Diphenylamine	Pest
G35	1241947	2-Ethylhexyl diphenyl phosphate	2-ethylhexyl diphenyl phosphate	Indu
G38	298464	Carbamazepine	Carbamazepine	PPCL
G40	128370	Butylated hydroxytoluene	BHT	PPCL
G42	131577	Benzophenone-3	Benzophenone-3	PPCL
G43	94133	Propylparaben	Propyl paraben	PPCL
G44	314409	Bromacil	Bromacil	Pest
G46	96764	2,4-Di-tert-butylphenol	2,4-DTBP	Indu
G47	132649	Dibenzofuran	Dibenzofuran	Indu
G48	77907	Tributyl acetylcitrate	ATBC	Plast
G49	2440224	Drometrizole	Drometrizole	PPCL
G50	93049	2-Methyoxynaphthalene	Nerolin	Indu

Table 4.6. Compounds detected by LC-MS screen not present in standard suites

Ranking	CAS Number	Analyte	Short name	Use code *
L06	298464	Carbamazepine	Carbamazepine	PPCL
L07	2971906	Clopidol	Clopidol	PPCL
L09	210880925	Clothianidin	Clothianidin	Pest
L11	723466	Sulfamethoxazole	Sulfamethoxazole	PPCL
L12	84057841	Lamotrigine	Lamotrigine	PPCL
L18	17254807	Chloridazon-desphenyl -methyl	CDM	Pest
L19	56038132	Sucralose	Sucralose	PPCL
L21	133855988	Epoxiconazole	Epoxiconazole	Pest
L22	188425856	Boscalid (Nicobifen)	Boscalid	Pest
L23	138261413	Imidacloprid	Imidacloprid	Pest
L25	120068373	Fipronil	Fipronil	Pest
L27	63741	Sulfanilamide	Sulfanilamide	PPCL
L28	115286	1,4,5,6,7,7-Hexachloro-5-norbornene-2,3-dicarboxylic acid	Chlorendic acid	Indu
L33	27203925	Tramadol	Tramadol	PPCL
L36	142459583	Flufenacet (Fluthiamide) (BAY FOE 5043)	Flufenacet	Pest
L38	5915413	Terbuthylazine	Terbuthylazine	Pest
L39	239110157	Fluopicolide	Fluopicolide	Pest
L41	107534963	Tebuconazole (Terbuconazole)	Tebuconazole	Pest
L42	153719234	Thiamethoxam	Thiamethoxam	Pest
L43	137586	Lidocaine (Diocaine)	Lidocaine	PPCL
L44	120983644	Desthio-prothioconazole	Desthio-prothioconazole	Pest
L45	2163691	Cycluron	Cycluron	Pest
L46	87674688	Dimethenamid (SAN 582H)	Dimethenamid	Pest
L47	422556089	Pyroxsulam	Pyroxsulam	Pest
L48	64902723	Chlorsulfuron	Chlorsulfuron	Pest
L49	21087649	Metribuzin	Metribuzin	Pest

Table 4.6 shows that the situation is similar for the LC-MS screen with 27 of 50 compounds detected not present in the standard suites. These are mainly pesticides, including TPs, and PPCL compounds.

4.3.2 Comparison of LODs

LODs for the top 50 compounds for the GC-MS screen are shown in Table 3.1 These are predominantly 0.01 µg/L with higher limits for four compounds, the industrial compound TMDD, the food additive BHT, and the plasticisers BBSA and DEHP.

LODs for the top 50 compounds for the LC-MS screen are shown in Table 3.2. These are predominantly an order of magnitude lower at 0.001 µg/L increasing for perfluorinated compounds, and also for the PPCLs sucralose, sulphanilamide and sulfamethoxazole, and the pesticides boscalid, trietazine and mecaprop.

The ranges of LODs for Environment Agency quantitative analytical suites are shown in Table 4.3. These are of a similar order of magnitude to the LC-MS method with higher limits for PAHs and difficult compounds, such as the pesticides chlormequat, glyphosate and metaldehyde.

4.3.3 Confidence

A third element must be the increased confidence in identification and quantification provided by the quantitative suites.

4.3.4 Case study on pesticides

Jenkins and Davy (2016) report on the comparison between quantitative suites and the target based LC-MS method for pesticides in six Catchment Sensitive Farming (CSF) examples. Key determinands in this study were propyzamide, metazachlor, atrazine, diazinion, ethofumasate, MCPP, simazine, mecoprop, carbetamide and 2,4-D.

They found that overall the methods produced comparable results. There was a higher degree of scatter in the relationship at lower concentrations indicating that one or both of the methods was less accurate for concentrations close to the LOD. The target based LC-MS method was less precise and it was assessed that there was an increased risk of false positives. However the target based method had a lower LOD for many of the compounds used in this example.

5 Conclusions and recommendations

This is the first study to assess robust summary statistics, using non-detects methods, for top 50 compounds for groundwater samples in England analysed by the target screening by GC-MS and LC-MS. Due to the high proportion of censored results in this type of data set, this approach is essential for future assessments to estimate summary statistics.

Targeted screening methods are particularly useful for surveillance purposes, i.e. assessing the occurrence of a broad range of emerging substances in groundwater, and are being (and should to continue to be) used to help prioritise ongoing monitoring activates in England and elsewhere in Europe.

The dominance of different groups of compounds differs for the GC-MS and LC-MS screen, and this reflects to a large extent the methodological differences, however, there are several frequently detected groups of compounds that are present in both suites including pesticides and pharmaceuticals. Five pesticides were detected in the top 50 for both screens.

The GC-MS results for the top 50 compounds are characterised by low frequency of detection (up to 1-10%), however max concentrations are high and are typically at 10-100 μg/L concentrations. LC-MS results for the top 50 compounds are characterised by much higher frequency of detections (10- 65%), however, maximum concentrations are typically at the sub μg/L concentrations. This difference to a large extent reflects the much lower LOD for the LC-MS method compared to the GC-MS method, and possibly the more limited spatial data coverage for the LC-MS method.

Spatially coherent results for many groups of compounds are found and can be related to different land use and/or sources of pollution as well as hydrogeological characteristics of aquifers in England, i.e. the degree of aquifer confinement as well as more karstic features in parts of the Chalk in England.

Pesticides, halogenated solvents and industrial compounds dominate the top 50 compounds for both LC-MS and GG/MS results, however, several emerging substances such as pharmaceuticals are represented in the top 50 in terms of frequency of detections and concentrations.

There is a much more limited LC-MS database so far compared to GC-MS data. The high frequency of detects are noteworthy, particularly for the LC-MS data set, >10% for top 50 compounds. This suggests that it would be beneficial to extend the spatial and temporal coverage of groundwater samples analysed in England, as well as Wales, Scotland and NI using this type of targeted approach.

A key priority for future work is assessing the potential risk to groundwater and groundwater dependant (eco)systems from hazardous substances.

Further work should be prioritised to assess the results for particular groups of emerging substances with high persistence and hazardous properties such as perfluorinated substances, pharmaceuticals – particularly anti-microbial substances, as well as neonicotinoids.

Further work to compare targeted screen data with results from dedicated suites, where there is an overlap in substances, is needed to fully understand the utility of the targeted screen data.

Appendix 1 Surface Water Watch List Updated June 2018

- 17-Alpha-ethinylestradiol (EE2) – steroid hormone TP
- 17-Beta-estradiol (E2), estrone (E1) - steroid hormone
- Macrolide antibiotics (erythromycin, clarithromycin, azithromycin)
- Methiocarb – pesticide -bird repellent, insecticide, acaricide and molluscicide
- Neonicotinoids (imidacloprid, thiacloprid, thiamethoxam, clothianidin, acetamiprid)
- Metaflumizone – veterinary insecticide
- Amoxicillin - antibiotic
- Ciprofloxacin - antibiotic

Deleted substances

- Diclofenac – pharmaceutical - nonsteroidal anti-inflammatory
- Oxadiazon and tri-allate - herbicides
- 2-ethylhexyl-4-methoxycinnamate (octinoxate)- sunscreen ingredient
- 2,6-di-tert-butyl-4-methylphenol

COMMISSION IMPLEMENTING DECISION (EU) 2018/840 of 5 June 2018 establishing a watch list of substances for Union-wide monitoring in the field of water policy pursuant to Directive 2008/105/EC of the European Parliament and of the Council and repealing Commission Implementing Decision (EU) 2015/495

Glossary

Additional compound names are given in full alongside their acronyms in Table 3.1 and Table 3.2.

BBSA	Benzenesulfonamide, N-butyl
BAM	2,6-Dichlorobenzamide
BHT	Butylated hydroxytoluene
BPA	Bisphenol A
CAS number	Chemical Abstract Service – a unique identifier for chemical
DWD	Drinking water directive 1998/83/EC
DEET	N,N-Diethyl-meta-toluamide
DEHP	Bis(2-ethylhexyl)phthalate
Emerging substance	Substances detected in the environment, but not included in routine monitoring programmes, whose fate, behaviour and toxicological effects are poorly understood
GC-MS	Gas chromatography-mass spectrometry (a laboratory analytical method)
LC-MS	Liquid chromatography-mass spectrometry
LOD	Limit of detection
MCPA	2-methly-4-chlorophenoxyacetic acid
MO	Micro-organic compound
Micro-organic compound	Organic compounds typically present at trace concentrations
PAH	polyaromatic hydrocarbons
Polyaromatic	Compounds with multiple ring structures
PFCs	Perfluorinated compounds
PFOA	Perfluorooctanoic acid
PFOS	Perfluorooctane sulfonate
PSD	Priority substances directive 2013/39/EU
PPPD	Plant Protection Products Directive 1107/2009/EC
Q-TOF	Quadrupole Time-of-Flight
REACH	Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH)
Screen(ing)	Refers to an analytical method that can detect a large number of compounds, rather than targeting a small suite of specific compounds.
SVHC	Substance of very high concern
SVOC	Semivolatile organic compounds
THMs	Trihalomethanes
TMDD	2,4,7,9-Tetramethyl-5-decyne-4,7-diol
TP	Transformation products, covering biotic and abiotic processes
TTT	2,4,6-Triallyloxy-1,3,5-triazine
UHD	Ultra-High-Definition
VOCS	Volatile organic compounds

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