Passive Sampling of Volatile Air Pollutants

Method development and validation of VOCs through passive air sampling by use of 3M 3500 diffusion monitors, measured by mass spectrometry gas chromatography

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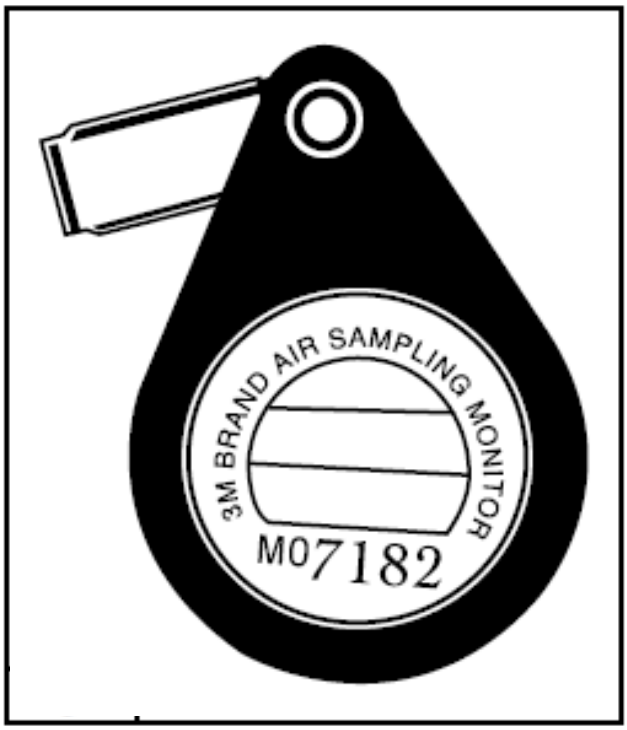

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ABREVIATIONS

SGS: Société Générale de Surveillance

VOCs: Volatile organic compounds

RPS: Rural planning services

IAQ: Indoor air quality

GC: Gas chromatography

MS: Mass spectrometry

LOD: Limit of detection

LOQ: Limit of quantitation

VVOCs: Very volatile organic compounds

SVOCs: Semi volatile organic compounds

PAS: Passive air sampler(s)

SR: Sampling rate

TDS: Thermal desorption system

SIM: Selective ion method

CMA: Compendium voor Monsterneming en Analyse

NEN: Nederlandse norm

CV_{RW}: Intra-reproducibility

SD: Standard deviation

CAS: Chemical abstracts service

MW: Molecular weight

Ppm: Parts per million

CF_T: Temperature correction factor

Atm: atmosphere (unit of pressure)

PGMEA: Propylene glycol monomethyl ether acetate

PGME: Propylene glycol monomethyl ether

SR_d: Sampling rate for a dynamic device

M: Mass of the sorbed analyte

D_{air}: Diffusion coefficient

A_d: Area of the sorption pad

L_d: Length of the diffusion path

D_g: Gas diffusivity

T: Absolute temperature in Kelvin

P: Absolute pressure in atmosphere

I_d: Collision integral for diffusion

V_2: The sum of all atomic values of a molecule

k: Boltzmann constant

W: Weighted amount of liquid injection

K_o: Sampling rate of the monitor

C: Average concentration analyte

t: Sampling time

RRF: Relative response factor

ISTD: Internal standard

SER: Sociaal-Economische Raad

ABSTRACT

An attempt was made to develop a method for the determination of volatile organic compounds (VOCs) in air by gas chromatography mass spectrometry (GC-MS) analysis and chemical sample desorption of the 3M 3500 passive diffusion sampler. The method included a complex mixture of 205 polar and non-polar compounds ranging from boiling points of – 24 ˚C to 286 ˚C. A selective ion method was established to achieve peak separation based on mass spectra for most compounds, after which the performance of the method was validated for the following parameters; limit of detection and quantitation and reproducibility. In addition, sampling rate and recovery coefficients were determined for every compound as these are crucial constants in the conversion calculation of analyte mass in air. After validation it was concluded that the method performance was insufficient for routine analysis and needed substantial improvements. Further research is required to develop and validate a functional method of analysis.

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1 INTRODUCTION

The research described in this report was performed for the company SGS's environmental laboratory, located in 's Gravenpolder. SGS, otherwise known as Société Générale de Surveillance, which was originally founded in Genève Switzerland in 1878 and has since been expanded to a prominent company with multiple laboratories and offices across the globe. They are known as the world's leading inspection, verification, testing and certification company. Their main objective is to surpass customer expectations and to always provide service with passion, integrity and innovation. For this reason, the company wishes to expand their current analysis of volatile organic compounds (VOCs) in air by the addition of roughly a hundred compounds, and compete with companies providing similar services, such as RPS laboratories and 3M. The current method of VOC analysis in air yields data for 86 compounds by use of passive air samplers (PAS), chemical desorption, and gas chromatography mass spectrometry (GC-MS) measurement.

The monitoring of organic environmental pollutants, by means of passive sampling, remains an ongoing challenge for the analytical chemist, in spite of its relatively long history (Namiesnik, Zabiegala, Kot-Wasik, Partyka, & Wasik, 2004). The company 3M, supplier of the badge-type sampler used in this research, is the leading company in VOC analysis by passive sampling. They have provided protocol-like documents to assist analysts in the procedure of analysis and method validation. Yet, a lot is still unclear in the field and no clear norms are set, which is why this research is of great importance. More research is required to develop a final successful method for the analysis of VOCs by use of passive sampling and GC-MS analysis.

Reasoning for the need of this analysis is the topic of indoor air quality (IAQ), which has represented a major concern for over three decades. It is well known that indoor air quality (IAQ) deterioration is caused by the occurrence of volatile chemicals, with the most important classes being VOCs and Carbonyls. VOCs cause health hazards due to their use in household products such as paints, varnishes, waxes, solvents and detergents (Sarigiannis, Karakitsios, Gotti, Liakos, & Katsoyiannis, 2011). It is important to monitor these compounds present in air to prevent adverse instant and long-term health effects. As mentioned, the monitoring of such compounds is often performed by the use of passive air samples with an activated charcoal sorbent layer, simple and inexpensive devices suitable for long term and individual exposure monitoring (Huang, Shan, & Xiao, 2018).

The aim of this research was to develop and validate a screening method for the analysis of 205 volatile organic compounds by means of passive air sampling on a 3M 3500 passive diffusion sampler, chemical desorption and GC-MS analysis. Two sets of GC-MS systems were used in the process of method development, yet only one was validated due to a shortage of time. After method development, the method performance was evaluated by the following quality parameters; recovery efficiency of sample desorption, linearity, limit of detection and quantitation and reproducibility. The method was set-up in consideration of the normatives MDHS 88, NEN 777 and the 3M manuals available.

The main research question is as follows,

What are the limitations of analysing 205 volatile organic compounds on a gas chromatograph mass spectrometry system after chemical sample desorption by use of carbon disulphide?

Which generated the following sub-question,

How does the addition of a secondary gas chromatography mass spectrometry system affect the scope and usability of the analysis?

2 THEORETICAL FRAMEWORK

2.1 VOLATILE ORGANIC COMPOUNDS

Volatile organic compounds (VOCs) are defined as organic molecules with a boiling point between 50 and 260 degrees Celsius (Sarigiannis, Karakitsios, Gotti, Liakos, & Katsoyiannis, 2011). An extension of this range can be made by the addition of very volatile organic compounds (VVOCs) with a boiling point range from 0 to 50-100 degrees Celsius and semi volatile organic compounds (SVOCs) with a boiling point range of 240-260 to 380-400 degrees Celsius (Molhave, 1991). Other VOC characteristics are their high saturated vapour pressure, low molecular weight and their high volatility at room temperature (Huang, Shan, & Xiao, 2018). VOCs could often be present in indoor spaces due to their high volatility and occurrence in common household products such as paints, varnishes, waxes, solvents, detergents and cleaning products (Sarigiannis, Karakitsios, Gotti, Liakos, & Katsoyiannis, 2011). The term VOC covers a wide range of compound classes such as aliphatic and aromatic compounds, amines, aldehydes, ketones, esters, ethers, alcohols acids and halogenated hydrocarbons (Huang, Shan, & Xiao, 2018). It is of great importance that these compounds are identified and quantified in the air, since many compounds can transfer to humans and have been linked to several adverse health effects. The severity of which can differ by compound concentration and the mixture of compounds present in the air (Ockenden, Jaward, & Jones, 2001). Long term health effects are caused by their toxic, carcinogenic and mutagenic effects (Huang, Shan, & Xiao, 2018). In addition, direct effects may cause skin irritation and neurotoxic effects (Molhave, 1991).

2.2 PASSIVE DIFFUSION MONITORS

Over the past three decades, advances in analytical methods for the determination of contaminant concentrations in air have been seen, since the passive air sampler (PAS) was introduced in the late 1970's, and has since been frequently used for monitoring of air pollutants such as VOCs (Bohlin, Jones, & Strandberg, 2007). Other than active air samplers, PAS can be used without air pumps and thus external force (Gosselink, Braun, Mullins, & Snowden, 1981). In addition, they are overall small and uncomplicated, easy to operate and transport. These characteristics make PAS more economical and practical to monitor VOCs when compared to active sampling techniques. As an alternative method to active sampling, PAS are especially suited for simultaneous large-scale measurement and long-term monitoring of individual exposure (Huang, Shan, & Xiao, 2018).The monitoring of individual exposure may be performed for either of the following reasons (Gosselink, Braun, Mullins, & Snowden, 1981):

1. To define a hazard by monitoring environmental exposure for an individual e.g. an employee.
2. To verify the safety of an individual e.g. an employee, in areas of exposure.

Due to the fact that PAS function without external force, they are dependent on either turbulent or molecular diffusion to absorb the analyte. As can be seen in figure 1, the analyte is transferred from the air or via the diffusive air flow, onto the sampled medium or sorbent (McLagan, et al., 2015).

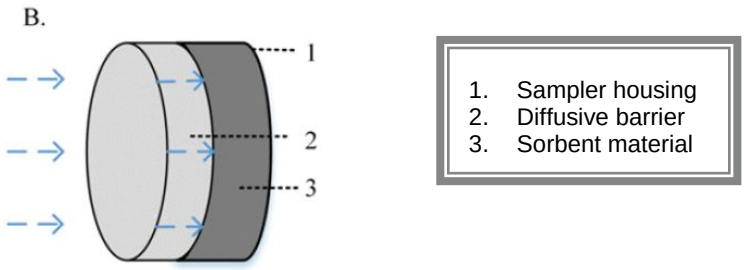

Figure 1. Schematics of a basic badge-type sampler, the blue arrows indicate the diffusive air flow (Huang, Shan, & Xiao, 2018).

The sorbent uptake of VOCs is based on vapour diffusion as described by Fick's first law, which assumes that the analyte concentration in the air remains constant while the mass of the sorbent pad will increase linearly until the maximum capacity or equilibrium is reached. This relationship only exists when it is assumed that the rate of desorption can be considered negligible when compared to the sorption rate (Gouin, Wania, Ruepert, & Castillo, 2008). In the linear sorption phase, the sampling rate in millilitres per minute could be derived by Fick's first law by use of the following equation,

[1]

$$SR_d = \frac{M}{t \cdot C} = \frac{D_{air}\, A_d}{L_d}$$

Where SR_d represents the sampling rate (SR) of a dynamic device, M equals the mass of the sorbed analyte in micrograms, t equals the sample time, C is the concentration of the analyte in air in micrograms per cubic meter, D_{air} is the diffusion coefficient in square centimetres per minute, A_d is the area of the sorption pad in square meters and L_d is the length of the diffusion path in centimetres (Huang, Shan, & Xiao, 2018). Sampling rate is a crucial parameter for quantitation of the analyte as it stands in direct relation to calculations needed to determine the exact analyte concentration in the air. Under ideal conditions, sampling rate is a constant value related to the diffusion coefficient and the dimensions of the sampler (Tolnai, Gelencser, Gal, & Hlavay, 2000). When the analyte concentration in air is constant it implies that ''M'' and ''t'' are linearly related in the so-called linear uptake phase (Huang, Shan, & Xiao, 2018). According to the 3M Sampling rate validation guide, sampling rates can be determined either experimentally or theoretically depending on the availability of recourses. In order to theoretically determine the sampling rate, the diffusion coefficient is calculated via the Hirschfelder equation,

[2]

$$D_g = \frac{BT^{3/2}\sqrt{1/M_1 + 1/M_2}}{P\, {r_{12}}^2\, I_d}$$

Where D_g represents the gas diffusivity in square centimetres per second, B equals $\left[10.7 - 2.46\sqrt{1/M_1 + 1/M_2}\right] \cdot 10^4$, T equals the absolute temperature in Kelvin (˚K), $M_{1,2}$ equals the molecular weight of molecules involved, P equals the absolute pressure in atmosphere (atm), r_{12} equals the collision diameter in ångström (Å), I_d equals the collision integral for diffusion, which is the function of kT/ε_{12}, which in turn is constructed of k equalling the Boltzmann constant ($1.38 \cdot 10^{-8}$erg/˚K) and Ɛ_{12}, which equals the energy of molecular interaction in ergs. To shorten the equation, as to make it more manageable, it can be simplified to the following equation,

[3]

$$D_g = \frac{\left(22.03 - 5.07\sqrt{0.0345 + \frac{1}{M_1}}\right)\left(\sqrt{0.0345 + \frac{1}{M_2}}\right)}{I_d(3.62 + 1.18\sqrt[3]{V_2})^2}$$

Where V_2 equals the sum of all atomic values of a molecule (Σ^{v}atomic), which can be derived from LeBas' Additivity Values and Rules (Albright, 2008; 3M, 1994) visible in table 1.

Table 1. LeBas values and rules of additivity.

LeBas Additivity Values and Rules - $V_2 = \Sigma^V$atomic	
Element	**Atomic values (V)**
Carbon	14.8
Chlorine	
* Terminal (R-Cl)	21.6
* Medial (R-CHCl-R)	24.6
Fluorine	8.7
Hydrogen	3.7
Bromine	27.0
Iodine	37.0
Nirogen	15.6
* In primary amines	10.5
* In secondary amines	12.0
Oxygen	12.8
* Doubly bound (C=O)	7.4
*Aldehydes & ketones	7.4
* Methyl esters	9.1
*Methyl ethers	9.9
* Higher ethers & esters	11.0
*Acids	12.0
* In union with S/N/P	8.3
Sulphur	25.6
Special rules:	
(1) Deduct 6 for a 3-membered ring	
(2) Deduct 8.5 for a 4-membered ring	
(3) Deduct 11.5 for a 5-membered ring	
(4) Deduct 15.0 for a 6-membered ring	
(5) Deduct 30.0 for a naphthalene ring	
(6) Deduct 47.5 for an antracene ring	

Since it has been shown that excellent empirical correlation can exist between sampling rate and calculated diffusion coefficients, sampling rates that cannot be determined experimentally, can be determined with an accuracy of ± 5% using the empirical relationship by use of data collected by 3M, displayed in the 3M Sampling rate validation protocol, see figures 2 through 4 (3M, 1994).

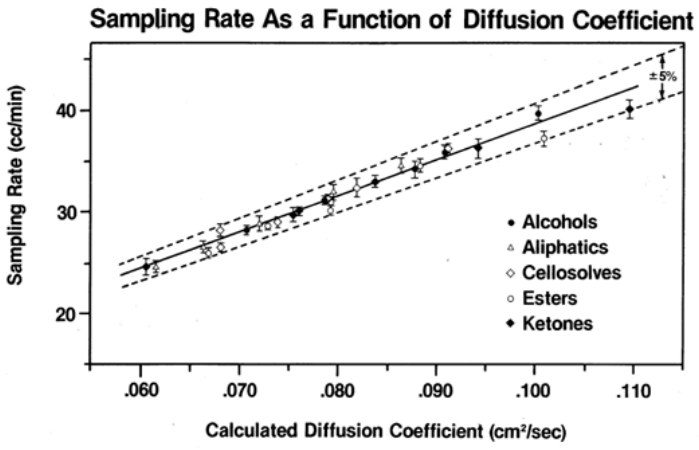

Figure 2. Empirical relationship between sampling rate in cc/min and the calculated diffusion coefficient in cm^2/sec for the compound classes alcohols, aliphatics, cellosolves, esters and ketones. (3M, 1994)

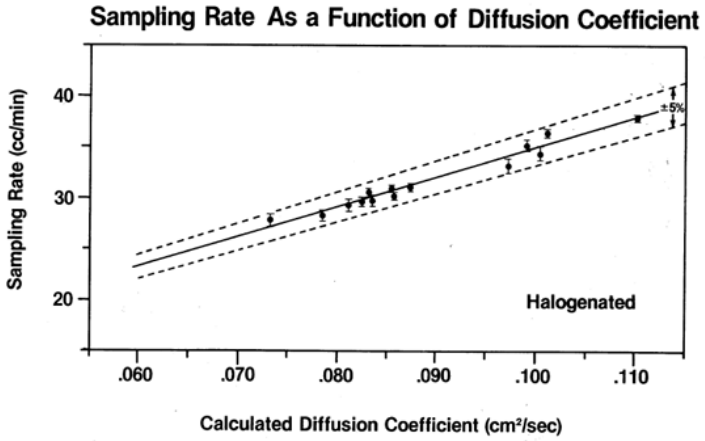

Figure 3. Empirical relationship between sampling rate in cc/min and the calculated diffusion coefficient in cm^2/sec for halogenated hydrocarbons. (3M, 1994)

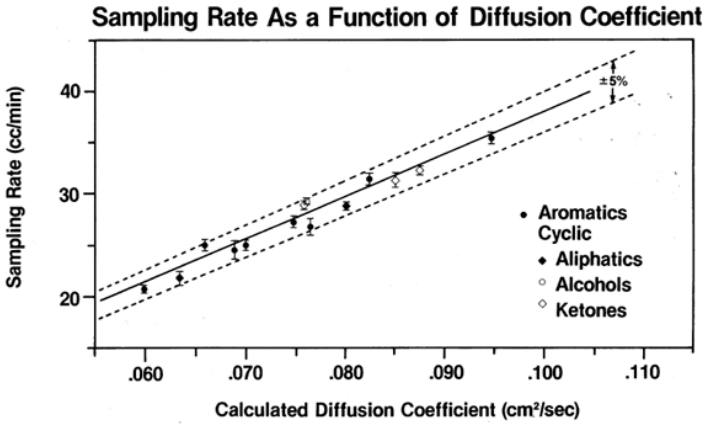

Figure 4. Empirical relationship between sampling rate in cc/min and the calculated diffusion coefficient in cm^2/sec for the compound classes aromatics and cyclic aliphatics, alcohols and ketones. (3M, 1994)

In addition to the sampling rate of the passive air sampler, the recovery efficiency of the sorbent is a crucial parameter to exact determination of pollutant concentration in the air and is necessary to know the efficiency of the desorption process (3M Science Applied to Life, 2019). According to the 3M Technical Data Bulletin, the determination of the recovery coefficient is performed experimentally through indirect spiking of the sorbent pad, by use of a tissue or filter paper. The recovery coefficient can be calculated by simply dividing the absolute amount of analyte recovered by the theoretical amount added in micrograms (MDHS 88, 1997).

Finally, the sorbent material, responsible for the uptake of analyte from air, can be considered the most important organ in the body of a PAS. It is required that the sorbent has a strong ability to sorb the analyte during the sampling period and can be efficiently desorbed, with a high recovery, in the process of analysis (Woolfenden, 2010), hence the crucial calculations of sampling rate and the recovery coefficient. The badges that will be used for this research are the 3M 3500 commercial-type badges, which were introduced to the market in 1978 and have since been used for both air quality and personal monitoring (Gosselink, Braun, Mullins, & Snowden, 1981). The sorbent medium used in 3M 3500 badges is active carbon, also called active charcoal, which is commonly used sorbents and is suitable for analysis of most VOCs. It is often preferred over other options due to its low cost, stable performance and its large uptake capacity (Huang, Shan, & Xiao, 2018).

With the sampling rate and recovery coefficient known, the sample concentrations could be determined by use of the following formulas,

[5]

$$c\left({}^{mg}/_{\mathrm{m3}}\right) = \frac{W \cdot A}{r \cdot t}$$

[6]

$$A = \frac{1000}{sampling\ rate\ ({}^{cc}/_{min})}$$

Where W equals the contaminant weight in micrograms, r equals the recovery coefficient and t equals the sampling time in minutes. Formula 5 is used to calculate the concentration of VOC's in air in the unit milligrams per cubic metre, and the corresponding calculation coefficient used is A, which is calculated by use of equation 6.

2.3 SAMPLE DESORPTION

As the sample is injected into the heated injection block of the GC using a syringe, and will enter the analytical column in gas phase, the desorption of active carbon will have to be performed using a liquid solvent (Lowell, White, & Taylor, 1970). Such a desorption solvent must poses the following characteristics; the solvent must be capable of stripping the active carbon sorbent from the analyte and do this with a high degree of efficiency, preferably with high reproducibility (Kennedy, Fischbach, Song, Eller, & Shulman, 1995). Carbon disulphide is a desorption solvent often used for the desorption of active charcoal commercial passive air samplers, it is a good solvent for non-polar compounds and elutes fairly early in on most common GC-columns due to its low boiling point of 46.3 ˚C. It generates a significant amount of heat when added to activated carbon, displacing other molecules. For this reason, it may be advised to perform the desorption process in a chilled environment for certain VVOCs, as some may be vaporized due to the heat generated (Harper, 2000). Desorption recoveries using carbon disulphide may differ with compound classes, especially when looking at compound polarity and reactivity. For example; non-polar non-reactive compounds such as toluene, hexane and 1,1,1-trichloroethane often show recoveries near 100%. Relatively non-polar yet more reactive compounds with stable double bonds, such as styrene, vinyl acetate and ethyl acetate, have recoveries dependent on the loading of the compound on active carbon. High loading of the compound per unit mass of charcoal shows sufficient recoveries, but as the loading decreases, so will the recovery, down to approximately 10 to 30%. Finally, polar compounds such as alcohols show poor solubility in carbon disulphide and would rather associate with other polar molecules (Harper & Fiorito, 1996). For this reason, 3M advises the use of a different desorption solvent for certain compounds, mostly alcohols and ketones. As alternative for carbon disulphide, methylene chloride is used as desorption solvent for these selected compounds as it is a slightly polar solvent other than carbon disulphide which is strongly non-polar (3M Science Applied to Life, 2019).

Both carbon disulphide and methylene chloride, used for chemical desorption, are highly toxic chemicals. For example, carbon disulphide has reactivity hazards such as spontaneous combustion when in contact with a surface with a temperature from 100 °C as well as violent chemical reactions with compressed air and oxidizing agents. In addition, symptoms of acute exposure are inflammation of the skin, blurred vision, headache, dullness and dizziness (Young, 2003).

2.4 MASS SPECTROMETRY GAS CHROMATOGRAPHY

To analyse all VOCs, approximately 205 compounds, an analysis method with high capacity, selectivity and sensitivity is required. Mass spectrometry gas chromatography (GC-MS), seems to be a fit analysis technique since it has a sample component capacity of 1-300, and a high sensitivity of 10^{-12} g. GC-MS is often used for multi-component analysis with high chances of co-elution. Gas chromatography has the ability of separating al components of a mixture and when combines with mass spectrometry, a technique is created to separate and identify all compounds (Karasek & Clement, 1988).GC-MS offers many advantages for VOC analysis and is often used in many such applications due to its aid in co-elution compound identification. Compounds that may co-elute on the GC column may still be separated based on their mass spectrum (Batterman & Chernyak, 2006).

The principles of a mass spectrometer are fairly simple, see figure 5 for a schematic of an MS. To elaborate, compounds separated by the gas chromatograph enter the mass spectrometer chamber via the interface, which connects the analytical column with the MS. The compounds are injected into a high vacuum where they can freely move, they will be fragmented into their constituent ions by the quadrupole (electron source), which emits a stream of electrons. The fragmented ions are then separated based on their mass by the magnet present and detected. A distinct pattern will be formed by which the compound can be identified, same as a humans fingerprint, these patterns are unique to each compound (Karasek & Clement, 1988).

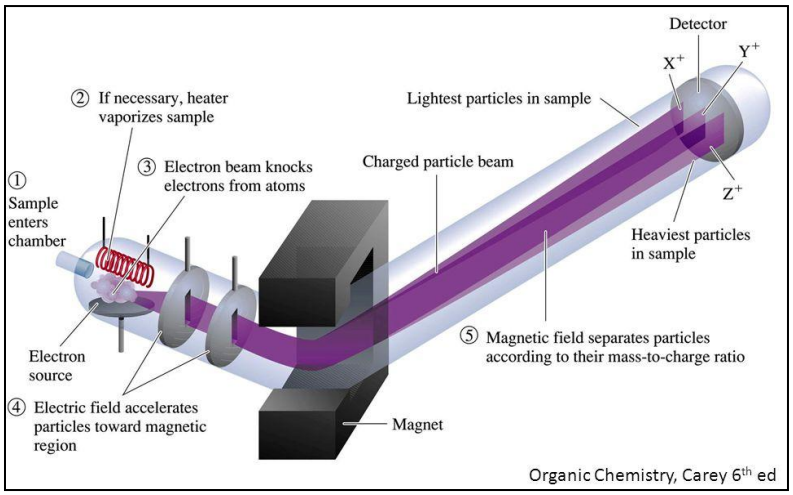

Figure 5. Schematic view of a mass spectrometer (Carey, 2006).

In addition to the MS's ability to identify compounds by mass, a selective ion method (SIM) can be applied, which will increase sensitivity and selectivity of the apparatus significantly (Batterman & Chernyak, 2006). With the use of a SIM, the analyst can select at which time during analysis which masses will be detected by the MS, other than when using a Full-scan method, where every detected mass is measured over the course of the entire analysis time. To view an example of the difference between a total ion chromatogram (full scan) and an extracted ion chromatogram (SIM method scan), see figure 6.

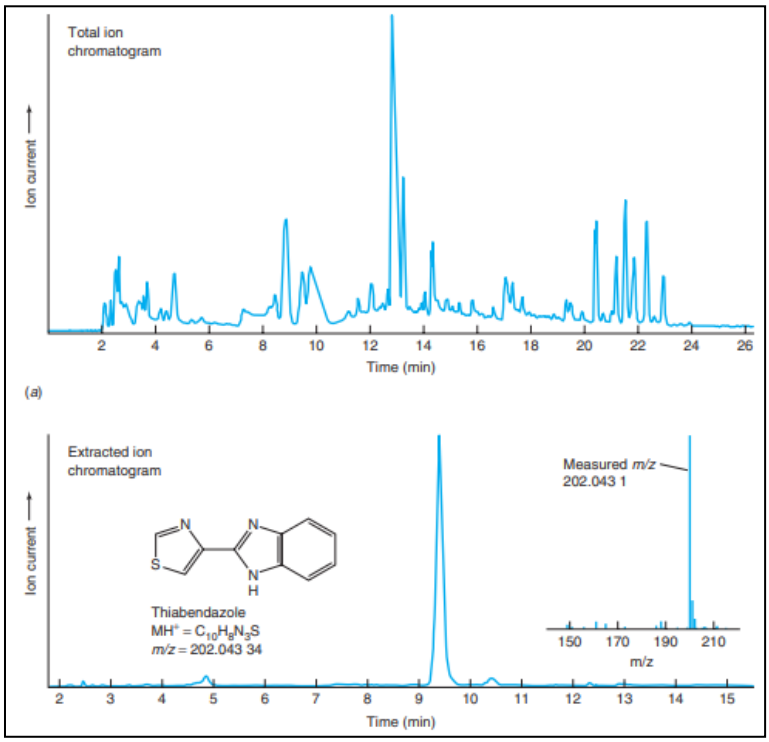

Figure 6. Two chromatograms, total ion (full scan) versus extracted ion (SIM) chromatogram where only mass 202.0431 was measured in a window (Quantitative Chemical Analysis 8th Edition).

2.5 GREEN ANALYTICAL CHEMISTRY

Green Chemistry is a major component in the development and growth of the scientific community in the aspect s of ‘’responsible care’’ and ‘’sustainable development’’. Making the reducing of hazards and risks an important criterion for the performance of either a product or process (Poliakoff, 2002). Green Chemistry movement has the aim to reduce hazards across all life-cycle stages and improve the efficiency and safety of chemical processes (Anastas & Engbali, 2010). The original 12 principles of green chemistry by Paul Anastas are mostly directed to sustainable developments, with a focus on industrial-scale processes in green organic chemistry. For this reason, they are not completely compatible with analytical chemistry processes.

Green Analytical Chemistry (GAC) emerged in the year 2000 and is still a relatively new area within the overarching field of Green Chemistry (Galuszka, Migaszewski, & Namiesnik, 2013). Analytical chemistry has played a major role in the environmental movement by detecting and monitoring environmental pollutants (Anastas & Kirchhoff, 2002), such as VOCs, with a main focus on transforming laboratory practices to increase safety and environmental friendliness of analysis. Which generates the following 12 principles expressed as the mnemonic ‘’SIGNIFICANCE, disrobed by Agnieszka Galuszka (Galuszka, Migaszewski, & Namiesnik, 2013),

S	-	Select direct analytical technique
I	-	Integrate analytical processes and operations
G	-	Generate as little waste as possible and treat it properly
N	-	Never waste energy
I	-	Implement automation and miniaturizing of methods
F	-	favour reagents obtained from a renewable source
I	-	Increase safety for the operator/analyst
C	-	carry out *in-situ* measurements
A	-	Avoid derivatization
N	-	Note that the sample number and size should be minimal
C	-	Choose a multi-analyte or multi-parameter method
E	-	Eliminate or replace toxic reagents

The main challenge in GAC, is to find compromise between quality of the results and improving environmental friendliness.

2.6 METHOD VALIDATION

For an analytical laboratory, the use of validated method is crucial for obtaining their accreditation and demonstrating their qualifications to the customer. Validation of a method is the act of investigating whether the analytical aim of the method has been achieved, which is performed by obtaining results with an acceptable uncertainty level conform with the norms/regulations to be upheld (Taverniers, De Loose, & Van Bockstaele, 2004). According to Pedro Araujo’s ‘’Key aspects of analytical method validation and linearity evaluation’’, the process of validation consists of five key elements; system qualifications, where the instrumentation, reagents and standards to be used are evaluated to see whether they are suitable for analysis. The choice of an appropriate sampling method to assure the selected sample is truly representative for the material in the aspect of meaningful statistical interferences. Sample preparation, which is critical for a successful method validation. When considering possible methods, it is important to consider these factors, sample matrix, analyte characteristics, concentration levels, sample size and the instrumentals. Analysis, which is related to the instrumentation to be used to acquire the qualitative and quantitative information with an acceptable level of uncertainty. When selecting the method of analysis, it is of great importance to consider the following factors, analyte characteristics and properties, sample matrix and thus a possible matrix effect, concentration levels and analysis time. Finally, data processing and evaluation, where the data acquired during validation is processed and evaluated to draw the appropriate

conclusions on whether or not the validation is successful and therefore sufficient to acquire accreditation for the company (Araujo, 2009).

*It is important to note that for this research, the exact methods and criteria of validation have not been determined. So, the parameters discussed in this section solely provide a broad range of information and possible methods to be used based on literature and company experience.

2.6.1 LIMIT OF DETECTION AND LIMIT OF QUANTITATION

Analytical procedures and their validity are often characterized by the following parameters, dynamic linear range, trueness, percent recovery and reproducibility. Another critical parameter for validation is the lowest concentration to be detected and quantified, otherwise known as the limit of detection (LOD) and limit of quantitation (LOQ). The LOD can be defined as the smallest amount of analyte that can clearly be distinguished from the blank measurement or background noise, and LOQ as the smallest amount of analyte to be quantified with a certain level of confidence. These two values may be determined via either of the following two approaches/methods, statistical, where results are based on the measurement of negative samples. Or the empirical approach where a range of sample dilutions are analysed to determine LOD and LOQ (Armbruster, Tillman, & Hubbs, 1994). David A. Arbruster, who compared the two methods in 1994, found the empirical method to provide a more accurate and realistic representation of the LOD/LOQ when compared to the analytical approach, which seemed to underestimate the values.

It is important to note that the limit of detection (LOD) and limit of quantitation (LOQ) should not be considered as absolute values but as estimate of the method's performance. As the results may vary from laboratory to laboratory, instrument to instrument etc (Kennedy, Fischbach, Song, Eller, & Shulman, 1995). When only applied in a single laboratory, the values can be considered as statistically verified data.

According to the MDHS88 and the Belgian state document EN 13528-2, the LOD and LOQ can be calculated via the following equations (13528-2, 2002; MDHS 88, 1997),

[7;8]

$$LOD = 3SD$$

$$LOQ = 6SD$$

2.6.2 LINEARITY

Linearity can be defined as the ability of a method to acquire measured data proportional to the analyte concentration (Taverniers, De Loose, & Van Bockstaele, 2004). The aspect of linearity is based on the belief that a straight-line or linear relationship exists between the in(x) and output(y) of a measurement. Functions generated from this relationship are either $y = f(x)$, when the base of the line crosses through zero, or $y = f(x) + \delta$ when it does not. The validity of linearity, although questionable, is often based on the value of the correlation coefficient (R) generated from a calibration curves' linear trend line, see equation 11 for the formula used for calculation of R^2 (Quantitative Chemical Analysis 8th Edition). It is assumed that a correlation coefficient close to 1.000 proves sufficient linearity, according to SGS regulations set in NEN norm 7777 and Daniel C. Harris, a value greater than 0.9950 is deemed a good fit for many purposes (Araujo, 2009; NEN 7777, 2003; Harris). When linearity has proved to be insufficient, the working range must be reduced to fit the linear range and generate a sufficient correlation coefficient (CMA/6/A, 2018).

[9]

$$R^2 = \frac{[\Sigma(x_i - \bar{x})(y_i - \bar{y})]^2}{\Sigma(x_i - \bar{x})^2\ \Sigma(\mathrm{y_i} - \bar{\mathrm{y}})^2}$$

To account for slight variation in either sample quantity or instrument response, an internal standard method is applied to the method of analysis. Where a known amount of a deuterium compound, for example benzene-D6, is added to the unknown sample. These compounds are often referred to as labelled compounds and correct the analyte concentrations for these variables that can occur from run to run (Quantitative Chemical Analysis 8th Edition). The correction factor generated from the internal standard method is the so-called relative response factor (RRF) and can be seen in equation 12 (NEN 7777, 2003).

[10]

$$RRF = \frac{Area\ ISTD}{Area\ compound\ of\ interest} \cdot 100\%$$

The internal standard method is used with all measurements during method development and validation, including linearity.

2.6.3 REPRODUCIBILITY

Reproducibility can be defined as the precision obtained by the execution of an number of measurements divided over a number of weeks (CMA/6/A, 2018), otherwise called intra-reproducibility with the sole demand of time-dependent intermediate precision. NEN 7777 states that the data must be collected over the course of a minimal of 4 weeks and 8 measurements and provides the following equation for intra-reproducibility (CV_{RW}),

[11]

$$CV_{RW} = \sqrt{\frac{\sum(SD_1)^2, (SD_2)^2, \ldots}{2n}}$$

Where SD is the standard deviation of a duplicate measurement and n is the number of measurements (duplicate measurements do not count as separate measurements) (NEN 7777, 2003).

3 METHOD

3.1 MATERIALS AND CHEMICALS

3.1.1 CHEMICALS

For the preparation of standards, many high purity organic compounds must be ordered. The standard C-VLU-LUCHT-A, with a concentration of 100 mg/L, contains 84 of the 193 compounds to be prepared and is provided by SGS. The remaining compounds must be made in separate stock standards with a concentration of 50 mg/L in methanol each. The following compounds were used to prepare these stock solutions: n-pentane , n-undecane , cyclopentane , 2-methoxyethylacetate , trans-decaline , ethylene glycol monobutyl ether , methyl isobutyl carbinol , isopropyl acetate 99+% , isopropyl glycidil ether 98+%, 2-propoxyethanol , 1,2,3,4-tetrahydronaphthalene 98% , 2-ethoxyethyl acetate 99% , 5-methyl-3-heptanone 94% , benzyl acetate 99% , butyl methacrylate , allyl alcohol 99+% , sec-amyl alcohol , Dimethylacetamide, benzyl chloride 99%, n-propyl acetate, ethylene glycol diethyl ether, isobutyl acetate, provided by Merck from Darmstadt, Germany. n-dodecane , n-tridecane 99+% , n-tetradecane 99% , α-pinene, 4-tert-butyl toluene, 2-methylbutane 99+%, 1,4-para-dioxane 99+%, n-butyl acetate, 2-methylcyclohexanone 98%, 2-butanone 99+%, n-butyl propionate 99+%, methyl acrylate 99%, 3-methyl-1-butanol 99%, 2-methyl-1-propanol 99+%, ethylene glycol dimethylether 99.5%, n-amyl acetate 99%, 3-methylcyclohexanone 97%, methyl isobutyl ketone 99.5%, 4-methylcyclohexanone 98%, dibutylether 99+%, cyclohexanone 99+%, ethylpropionate 99+%, isoamyl acetate 99+%, ethyl acrylate 99.5%, methyl cellosolve 99+%, Isophrone 97%, 1-methyl-2-pyrrolidinone 99.5%, ethylene chlorohydrin 99+% and furfural 99%, provided by Acros Organics from Geel, Belgium. n-pentadecane 99%, n-hexadecane 99%, 2,4-dimethyl-3-pentanone 98%, methylal 98%, 1,2-diethylbenzene, isopropyl glycol 99%, methyl butyl ketone 98%, 2-methyl-2-butanol 98%, mesityl oxide 90+%, Propylene glycol monomethyl ether acetate (PGMEA) 99%, Diethyl ketone 99%, 3-Heptanone 98%, 4-Hydroxyl-4-methyl-2-pentanone 98+%, 2-Butoxy ethyl acetate 98%, 3-Pentanol 98+%, epichlorohydrin 99%, 2-Ethoxyethanol 99%, Methyl amyl ketone 99%, diisobutyl ketone 90+%, Ethylene glycol diacetate 97%, 3-Methyl-2-butanone 98%, n-propanol 99+%, tetrahydrothiophene 98%, trans-4-methylcyclohexanol 98%, 1,4-diisopropylbenzene 98%, dipropyl ketone 98%, methyl propyl ketone 99%, methyl isoamyl ketone 99%, dichloroethyl ether 99%, n-amyl alcohol 99+%, acrylonitrile 99+%, furfuryl alcohol 98%, sec-butyl alcohol 99%, propylene glycol monomethyl ether (PGME) 99+%, tert-butyl alcohol 99+% and diethylene glycol diethyl ether 99%, provided by Alfa Aesar, from Heysham, Lancashire, United Kingdom. cyclohexene, D-limonene, 2,4-dimethylpentane and α-methyl styrene, provided by Thermo Fisher Scientific from Dreieich, Germany. 4-Vinyl-1cyclohexene , Methyl cyclopentane, 1-Bromo-3chloropentane 99%, Butyl acrylate, Butyl glycidyl ether 95%, cis-2-Methylcyclohexanol 98%, Dipropylene glycol methyl ether 97%, trans-2-Methylcyclohexanol 99%, Cyclopentanone, cis-Decaline 99%, isobutyl benzene 99%, Cyclohexanol 99%, n,n-Dimethyl formamide 99.8%, provided by Sigma Aldrich from St. Gallen, Switzerland. Isooctane, Ethyl acetate 99.8%, provided by VWR Chemicals from Radnor, Darmstadt, Germany. 2,2-Dimethylbutane, 2-Methylpentane and Methylcyclohexane 99.5%, 1,3-Butadiene (100 µg/ml in methanol), provided by DR Ehrenstorfer from Augsburg, Germany. Benzyl alcohol 99+% and n-Butyl alcohol 99.7+%, provided by Honeywell from Düsseldorf, Germany. Cyclohexane, provided by Fluka Analytical from Seelze, Germany. Cis-4-Methylcyclohexanol 98%, provided by Combi-Blocks from San Diego, California, United States. 1,3- Diisopropenylbenzene 96%, provided by Toronto Research Chemicals inc., from Brisbane, Ontario, Canada (ordered via LGC Standards GMBH, Wesel, Germany) and acetone 99.9+%, provided by Biosolve from Valkenswaard, Netherlands.

Ampoules used for preparation of the calibration standard C-VLU-LUCHT-GCMS-G are R-683, at 2000 mg/L provided by Chem lab-Analytical, Zedelgem, Belgium. R-838 at 2000 mg/L, provided by Accu Standard, Huddersfield, United Kingdom. R-840 and R-841, both at 2000 mg/L and provided by Restek Corporation, Bellefonte, Pennsylvania, United States (ordered via distributer Interscience B.V., Breda, Netherlands). Test ampoule for VVOC's, the R-434 VOC mixture at 200 mg/L, manufactured for Agilent by Ultra Scientific Inc, United States.

Solvents used for the preparation of standards are, carbon disulphide with and internal standard in a concentration of 1 mg/L, labelled as extraction solvent with the name/code C-VLU-LUCHT-GCMS-B, provided and prepared by SGS Netherlands B.V., location 's Gravenpolder, Netherlands. Carbon disulphide 99.9+% and methanol 99.9+% provided by Honeywell from Düsseldorf, Germany. Methylene chloride 99.9%, provided by Biosolve from Valkenswaard, Netherlands.

3.1.2 MATERIALS

3M 3500 active charcoal passive diffusion monitors, provided by 3M© Science Applied to Life, Bracknell, United Kingdom.

GC-MS system 1:

Agilent 6890 series GC system paired with an Agilent 5973N Network MS detector, provided by Agilent Technologies, Amstelveen, Netherlands. The analytical column installed is the Rxi-624SilMS, with dimensions 60m x 0.32mm x 1.8µm, provided by Agilent Technologies, Amstelveen, Netherlands. The software used to run the GC-MS system is Xcalibur, Thermo Fisher Scientific Inc., Dreieich, Germany.

GC-MS system 2:

DSQ ll Single Quadrupole GC-MS: Focus GC, paired with a DSQ ll MS system, both provided by Interscience – Thermo Electron, Dreieich, Germany. The analytical column installed is the VF-1ms, with dimension 60m x 0.32mm x 1.0µm, provided by Agilent Technologies, Amstelveen, Netherlands. The software used to run the GC-MS system is MSD ChemStation D.02.00.275, Copyright Agilent Technologies 1989-2005, Amstelveen, Netherlands.

Software used for data analysis:

To view all compounds Q- and secondary mass peaks, the program Tracefinder version 3.2.513.0 is used, provided by Thermo Fischer Scientific Inc., Copyright 1991-2014, Dreieich, Germany. To view the complete chromatogram, the program Qual Browser Thermo Xcalibur, version 3.0.63 is used, provided by Thermo Fisher Scientific Inc., Copyright 1998-2013, Dreieich, Germany. The software which provides a large library of mass spectrums is NIST MS Search, Version 2.2, provided by FairCom Corporation, Portions copyright 1984-1996, Gazzaniga, Italy.

3.2 METHODS

3.2.1 EXTRACTION AND ANALYSIS

Tables 2 and 3 display the instrumental conditions for VOC analysis on systems 1 and 2. All 205 Volatile organic compounds have been identified by their retention time and mass spectra at full scan measurement on both systems. To continually identify compound peaks in Tracefinder after selective ion measurement (SIM), three masses are selected from their unique spectra, a Q-mass and 2 qualifier masses. The Tracefinder software allows for peak identification with every analysis by depicting the Q-mass and the ratios in which the qualifier masses exist. This ratio can vary slightly but must always agree with that of the compound in the calibration standard and library.

SIM methods have been developed for both systems and allow for selective mass detection and increased sensitivity, as can be seen in 2.4, figure 6. The SIM methods for system 1 and 2 can be found in Appendix II, tables 2, 3 and 4.

Table 2. GC-MS operating parameters for VOC analysis on system 1.

Injector	Split, 200˚C, split ratio 10:1, split flow 19.6 ml/min
Column	Agilent Rxi-624 Sil MS column at 60 m length, 0.32 mm inner diameter and 1.8 µm film thickness Ultralow-bleed mid-polar column, made up of 6% cyanopropyl/phenyl and 94% polydimethylsiloxane
Carrier	Helium, 2 ml/min
Temperature program	5 minutes at 35˚C, increase at a rate of 6.0˚C/min to 250˚C (no hold time), increase at a rate of 25˚C/min to 280˚C and hold for 2.97 minutes for a total run time of 45 minutes
Injection volume	2 µl
Mass spectrometer	Quadrupole 150˚C, MS source 230˚C

Table 3. GC-MS operating parameters for VOC analysis on system 2.

Injector	Split, 225˚C, split ratio 10:1, split flow 20 ml/min
Column	Agilent VF1ms column with dimethylpolysiloxane phase, providing increased sensitivity. 60 m length, 0.32 mm inner diameter and 1.0 µm film thickness Highly inert and non-polar
Carrier	Helium, 2 ml/min
Temperature program	5 minutes at 35˚C, increase at a rate of 7.5˚C/min to 300˚C (no hold time), increase at a rate of 25˚C/min to 325˚C and hold for 3.67 minutes for a total run time of 45 minutes
Injection volume	1 µl
Mass spectrometer	Transfer line 200˚C, MS source 250˚C

The 3M 3500 passive diffusion monitors used as sample medium are an axial badge-type sampler which consists of a permeable membrane, and a disk-shaped activated charcoal pad of approximately 180 mg which is assembled in a disk-shaped holder, view figure 7.

Figure 7. 3M 3500 passive diffusion sampler; 1. Permeable membrane, 2. Plastic ring, 3. Elution cap, 4. Activated charcoal disk (sorbent), 5. Spacer plate.

To extract volatile organic compounds from the sorbent (activated charcoal), chemical desorption is performed. First, the white film and plastic ring are detached from the monitor, to expose the sorbent pad. Then, 2 ml of the desorption, solvent (carbon disulphide*) with 1 mg/l internal standards, is transferred onto the sorbent pad. The elution cap, point 3 in figure 7, is placed onto the monitor and pressed secure to assure a tight seal. The monitor is placed onto an automatic shaker for 30 minutes, to agitate the monitor and bring all volatile organic compounds into solution. After 30 minutes, the solvent solution is transferred to a GC-MS insert vail (0.3 ml) and is ready to be placed in the auto sampler. Due to the volatile character of the solutions, samples and standards, all are placed in the GC-MS auto sampler and analysed immediately. Samples are partially stored in the freezer when a large number must be analysed, reason for this is the 45-minute run time. The length of the analysis can cause samples and standards to gradually decrease in concentration and thus detector response, though internal standards can partially correct for this, prevention is preferred because of the high number of compounds and their diversity in volatility.

*With the development of this method, a choice was made to only use carbon disulphide as a desorption solvent due to a lack of time.

3.2.2 STANDARD PREPARATION

In preparation for the calibration standard, a series of stock standards are first prepared. The calibration standard is composed of the following stock solutions, an ampoule with 1,3-Butadiene in a concentration of 1000 mg/l in methanol, the ampoules R-838, R-840, R-841 and R-683, with a concentration of 2000 mg/L in methanol, to view the compounds present in every ampoule see Appendix ll, table 5. In addition to these ampoules, 7 stock standards are prepared by hand by dilution of pure chemicals. These seven standards are needed to bring 119 compounds, not present in any of the ampoules, into solution. Due to the number of compounds, they are split into the following categories; aliphatics, halogenated compounds, ketones, esters, alcohols, cyclic/aromatic compounds and any excess compounds, see Appendix ll, table 6. for the composition of all stock standards and the exact concentration of each individual compound. To prepare the stocks, transfer 25 µl of pure chemical into a 10 ml volumetric flask partially filled with methanol. It is important to transfer the analyte directly into the solvent, due to its volatile character. Do this for every compound and fill up to the mark with methanol. Transfer the stock solutions to 10 ml dark glass bottles and store them in the freezer. Same as the ampoules, the 7 stock standards prepared have a concentration of 2000 mg/l in methanol.

To prepare the calibration standard with a concentration of 100 mg/l in methanol, all stock standards are combined. 500 µl of R-838, R-840, R-841, R-683, stock standards 1 through 7 and 100 µl of 1,3-Butadiene solution are transferred into a 10 ml volumetric flask and filled up to the mark with methanol. Divide this solution into 1.5 ml darkened glass vials with screw cap and store them in the freezer. View Appendix ll, table 7. for a schematic overview of preparation of the calibration standard. Stock and calibration standards can be stored into the freezer for a period up to six months.

To prepare a standard for analysis with a concentration of 1 mg/l in carbon disulphide, transfer 990 µl of carbon disulphide into a 1.5 ml GC-MS vail. To this, transfer 10 µl of the calibration standard directly into the solvent. Mix the solution by use of a glass pipette and divide over three GC-MS insert vails of 0.3 ml. This standard is prepared fresh for every analysis and cannot be stored for longer periods of time without the risk of analyte reduction.

3.2.3 SAMPLING RATE AND RECOVERY EFFICIENCY

The sampling rate, in cc/minute, can be determined both experimentally and theoretically. Due to a lack of recourses, sampling rate is calculated theoretically via the 3M sampling rate validation protocol. According to this protocol, sampling rate is determined by first calculating the diffusion coefficient by use of equation 3, an example calculation can be found in Appendix ll. With the diffusion coefficient value, the sampling rate can be derived by use of the empirical relationship between the sampling rate and the diffusion coefficient. Figures 2,3 and 4 in section 2.2, show 3 curves, all for different compound classes, so it is important to first determine the compound class of the compound of interest. Since these figures do not include a formula for the line, the raw data must be plotted manually using Excel to generate a function of the line. This raw data and the curves generated can be found in Appendix ll, table 9 and figure 1. To view all sampling rates, provided by 3M and theoretically calculated, see Appendix ll, table 10.

Other than the sampling rate, the recovery coefficient is determined experimentally. This is done by the addition of a known amount of analyte to the monitor at 3 levels; 0.1 mg/l, 2.0 mg/l and 10 mg/l, in

triplicate (n=3). The standard that is used for sample spiking is the calibration standard (100 mg/l) and is added in the following quantities for each level; add 2 µl for the lowest level of 0.1 mg/l, 40 µl for 2 mg/l and 200 µl for 10 mg/l. To assure the analyte is evaporated and equally distributed onto the sorbent material, an ashless/white ribbon filter paper with a diameter of 2.5 cm is used. The spiking procedure is as follows; select a blank 3M 3500 monitor and remove the plastic ring and white film. Place the filter paper directly onto the spacer plate to separate it from the sorbent. Snap on the elution cap and snap it shut to assure a tight seal. Inject the standard solution by use of a syringe through the centre port onto the filter paper. Close the port and allow the monitor to sit for a minimum of 16 hours at room temperature. Afterwards the monitor is extracted and analysed as described in section 3.2.1. After elution, the monitor is stored in the freezer. Recovery efficiency is calculated after analysis by dividing the amount recovered, by the theoretical amount and is expressed in percentages. A recovery efficiency >75% is desirable, any compounds resulting in a value <75% are analysed as semi-quantitative in this method.

3.2.4 TIME WEIGHTED AVERAGE CONCENTRATION

During the method validation, the unit that is used to express concentration is mg/l, since all samples are created by spiking of a liquid standard. This is done to simplify all calculations and keep results universal for every compound. Non-the-less, the unit in which the amount of analyte in air is expressed is mg/m^3. To convert the concentration in mg/l to mg/m^3, multiple variables are required, such as sampling rate, unique to every compound, used to calculate the calculation coefficient by use of formula 6. The recovery coefficient, determined for every compound, the absolute amount of analyte in micrograms and the sampling time in minutes. The time weighted average concentration in mg/m^3 is calculated by use of formula 5.

3.2.5 VALIDATION REQUIREMENTS

For this method of analysis, no set norms are in place to set strict validation requirements. For this reason, the 3M sampling and analysis guide, the 3M sampling rate validation protocol, MDHS 88, NEN 777 and EN 13528 were used as references. NEN 7777 (normative on method development and validation) requires for a validation period of a minimum of four weeks with a minimum of 8 measurements per validation parameter. GC-MS system 1 was validated for as many compounds as possible.

Linearity was determined by analysis of a series of standards in a concentration range of 0.1 to 10 mg/l in carbon disulphide on two GC-MS systems. All data point areas were corrected for their corresponding internal standard. The acceptable linear range has a correlation coefficient <0.995 and a minimum of 5 data points, as required by NEN 777.

The limit of detection and quantitation was determined by sample spiking at the concentration level 0.1 mg/l, since this is the reporting limit currently used in VOC badge-type analysis. The number of data points for the limit of detection and quantitation is ten (n=8). The calculations used for the limit of detection and quantitation are equations 9 and 10, where the LOD equals 3 times the standard deviation and the LOD equals 6 times the standard deviation.

Reproducibility is determined at two levels; 2.0 and 10.0 mg/l by sample spiking. The number of data points collected is ten (n=8), where a variance coefficient of maximum 20% is required for satisfactory results (OK/NOK).

4 RESULTS AND DISCUSSION

4.1 METHOD DEVELOPMENT AND OPTIMIZATION

4.1.1 METHOD DEVELOPMENT

By use of full scan measurement on GC-MS systems 1 and 2, all compound retention times were determined. To view all data on the elution order of the system, see Appendix lll, table 11. As expected, the elution of all compounds on a single analytical column proved to be a great challenge due to the scope of the method. Figure 8 provides some insight in the extent of co-elution which occurs in this method, showing a small section of a total ion chromatogram. Even with the use of an ultra-low bleed, mid-polar column and a run time of 45 minutes, it proved to be impossible to achieve base-line separation for most compounds. To help solve the issue and provide increased peak separation, the SIM method was developed, carefully selecting three masses for each compound.

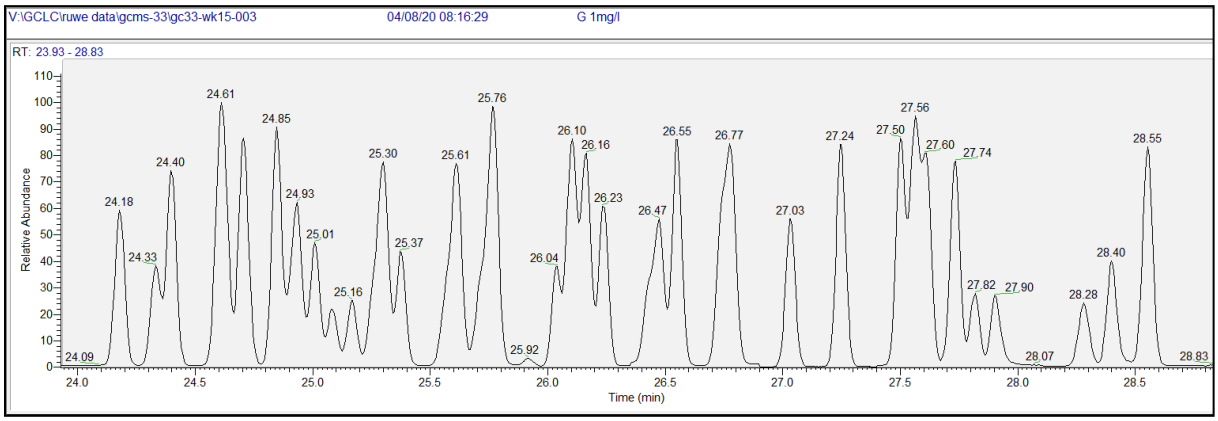

Figure 8. Zoomed-in view of a total ion chromatogram from RT 24.00 to 29.00 minutes on system 2, column Rxi-624. This chromatogram was generated by measurement of the calibration standard at 2 mg/l.

However, the use of a SIM method did not prevent all compounds from co elution. Reason for this are the similarities in mass spectrums between many of the 205 volatile organic compounds. A large percentage of compounds in the method are aliphatic, which mostly share the following masses in a spectrum; 41, 43, 56, 57, 71 etc. Still, this does not have to be an issue when a compound of interest has additional, more specific and higher masses. Generally mass fractions on the higher end of the spectrum tend to be more specific. However, if a compound only had these masses to choose from, it was challenging to generate base-line separated peaks when co elution occurred. The high occurrence of co elution decreases the probability percentage of some compounds. During method development, an attempt was made to increase probability by measurement of the added compounds in groups of 4 - 5 compounds. With this method, all retention times were determined accurately and with confidence. So, when looking at the retention times of each compound, these poses a high probability percentage. Unfortunately, this was decreased by co elution and similarities in mass spectra. A great example of this are the two compounds cumene and 3-ethyltoluene, which co elute at 23.39 minutes on system 1. It can be seen in figures 9 and 10 that these compounds share almost identical mass spectrums, which prevented them from being separated by mass selection.

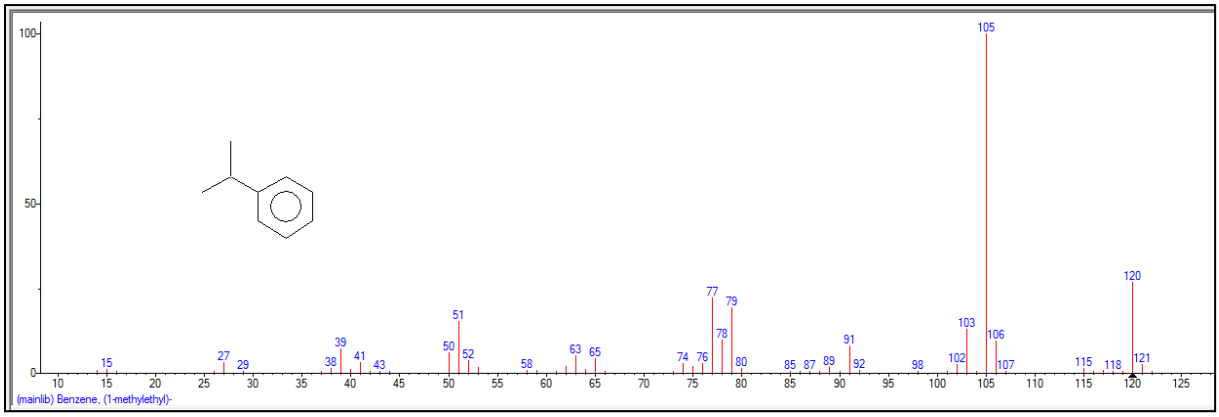

Figure 9. Mass spectrum of Cumene, RT 23.39 on system 2, column Rxi-624. (NIST MS Search 2.2)

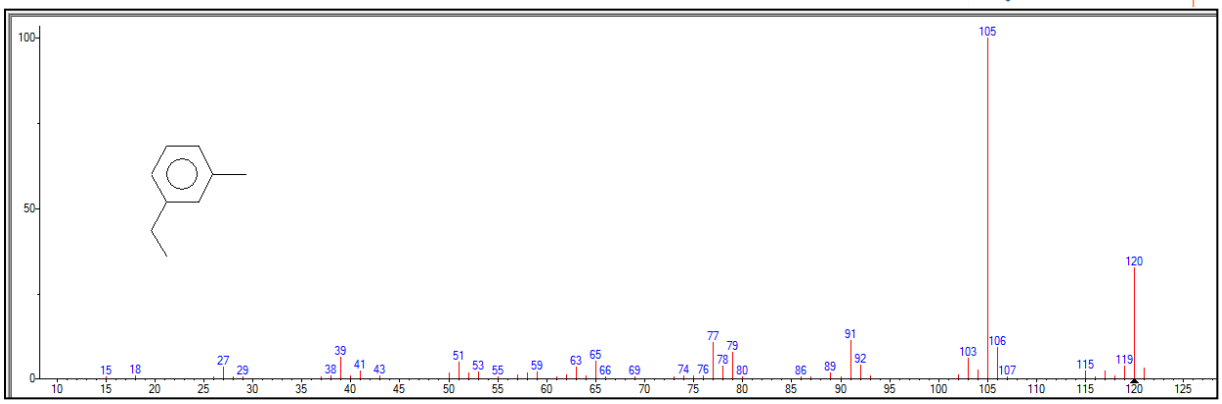

Figure 10. Mass spectrum of 3-Ethyltoluene, RT 23.39 on system 2, column Rxi-624. (NIST MS Search 2.2)

Another solution for co elution could be to view the two compound peaks as one, same as is done with para- and meta-xylene and report the sum. This could be a fit solution for cumene and 3-ethyltoluene, since they are so similar.

System 2 was initially introduced as a tool to possibly achieve sufficient separation, where system one did not. Unfortunately, due to a lack of time, not all data from the system could be analysed and processed in this report. However, method validation was performed for the system and two crucial compounds could be baseline separated on the VF-1 analytical column, where the Rxi-624 could not. These two compounds are allyl alcohol and isooctane. On system 1, acrylonitrile co-eluted with the solvent peak of carbon disulphide and could therefore not be detected. Isooctane is a compound which is used as a rinsing solvent on system 1 and therefore yields a rather large peak which is present with every injection. System 2 uses a different rinsing solvent which is not a compound of interest, acrylonitrile, therefore isooctane could successfully be analysed on the second system. Figure 11 shows the peaks of the two compounds, three peaks of each. Their Q-mass and confirming ions, all baseline separated.

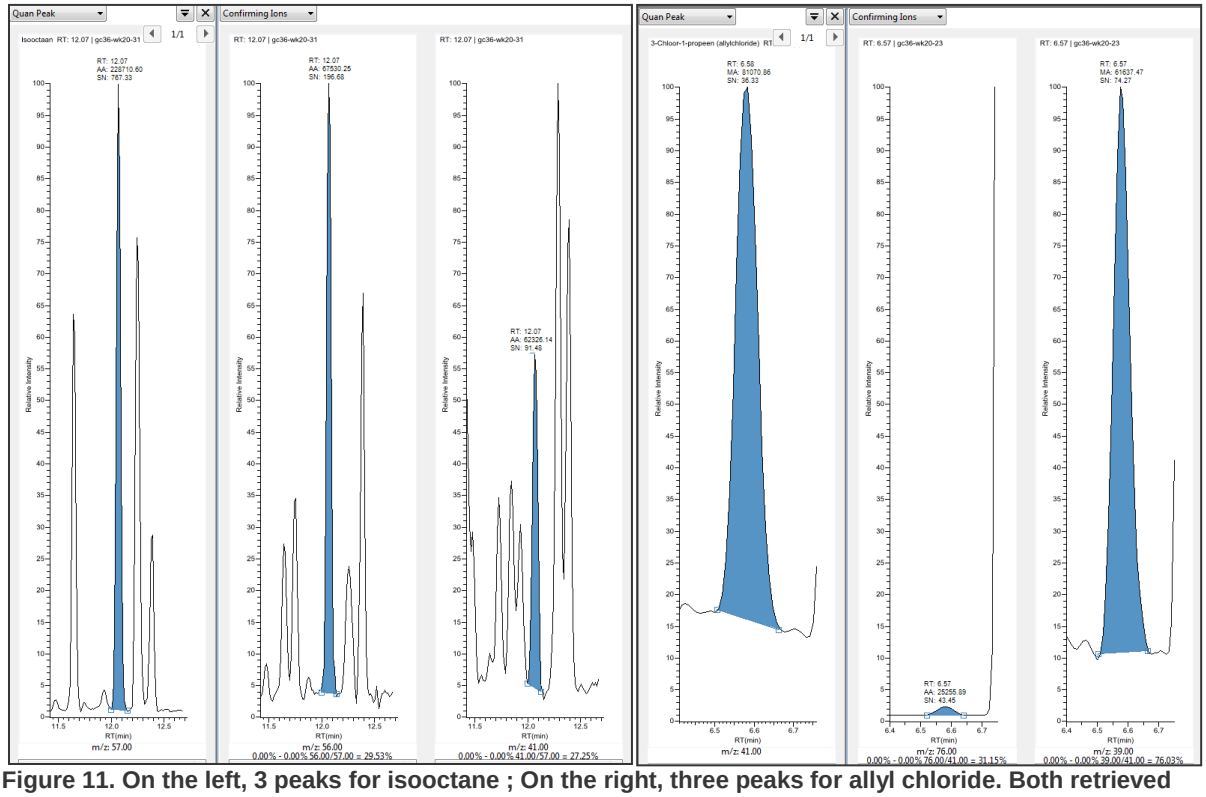

Figure 11. On the left, 3 peaks for isooctane ; On the right, three peaks for allyl chloride. Both retrieved from measurements performed on GC-MS system 2 with analytical column VF-1.

4.1.2 GREEN ANALYTICAL CHEMISTRY

As mentioned in the theoretical framework, the greatest challenge in green analytical chemistry (GAC) is to fiend compromise between the quality of results and improving environmental friendliness (Galuszka, Migaszewski, & Namiesnik, 2013). The method of chemical desorption can cause some concerns in regard to environmental friendliness and analyst safety. To focus on some of the principles of GAC, these are some positive aspects of the method of sample preparation and analysis; By preparing a highly concentrated stock solution of 100 mg/l, and preparing standards freshly in small volumes each analysis, little waste is generated. The waste which is generated is handled correctly at the SGS laboratory. The use of GC-MS insert vials also minimizes the waste of samples and standards by approximately 80%, since their maximum volume is 0.3 ml instead of 1.5 ml (standard GC-MS vial). Sample size is also fairly small in this method, since only 2 ml of carbon disulphide is added for chemical desorption, of which a small fraction is used for analysis. Of course, this does generate some sample waste, yet the possibility of redoing the analysis must also be considered. This is how compromises exist between quality and environmental friendliness.

Some negative aspects of the method are the toxic reagent and the analyst's safety. Chemical desorption by use of the solvent carbon disulphide is not ideal, considering its high toxicity and repugnant odour. Some measures were taken ventilate critical areas, such as fume hoods and point suction above the auto sampler. Some suggestions could be made to replace this method of sample extraction, but raises the question whether quality, cost and efficiency of the analysis is worth sacrificing for an improvement in green chemistry.

4.1.3 RECOVERY EFFICIENCY

Literature suggests that for the desorption of a mix of polar and nonpolar volatile organic compounds, no ideal solvent exists. MDHS 88 generally recommends that carbon disulphide be used as desorption solvent (MDHS 88, 1997). While carbon disulphide is an excellent solvent to use for many hydrocarbons, it yields poor recovery for polar compounds such as alcohols, ketones and ethers (Lopes, 1997). In addition, the loading dependency of the recovery efficiency could cause difficulties in quantitation of the analysis (Beck, Stock, & Whitehead, 1990). These statements were proven to be true during determination of the recovery coefficients, since the choice was made to use carbon disulphide as desorption solvent and not look into the use of methylene chloride, which according to 3M would increase recoveries in polar compounds (3M Science Applied to Life, 2019). This choice was made based on time-management and a lack of resources. The use of only carbon disulphide as desorption solvent caused a number of compounds to have a recovery of near 0%. This was the case for the following seven compounds; 1-Methyl-2-pyrrolidon , dimethyl formamide, ethylene glycol monobutyl ether , dipropylene glycol methyl ether , methylal, mesityl oxide and n,n-dimethylacetamide. As a result, these compounds could not be included in the analysis until more desorption solvent options are explored and tested. A recovery lower than 75% is not an issue, since it is accounted for in the conversion calculation from mg/L to mg/m^3 by use of equation 5. Yet, improvements in recovery efficiency must be made for those compounds which cannot be quantified after carbon disulphide desorption.

The high volatility of the very volatile organic compounds (VVOCs) with boiling points of 50 degrees Celsius or lower, caused some additional challenges. VVOC's are very quick to evaporate and this caused high variation from one measurement to another. Also, their high volatility causes, in some compounds, recoveries lower than 75%, in some even lower than 50%. Figure 12 is a visual representation of the VVOC recoveries at a theoretical concentration of 2 mg/L. It can be seen that high variation exists between measurements and compounds. Standard deviation bars were added to show the variation from measurement to measurement, some VVOC's proved to be more stable than others. This could be related back to their boiling points. For example, 1,1-dichloethene has a boiling point of 32 degrees Celsius, while chloromethane has one of minus 24.2 degrees Celsius. These are two very extreme opposite, but it does demonstrate the relationship between their variation and boiling point. When comparing the VVOC results with figure 13, which displays the volatile organic compounds recovery results, there remains much variation in recoveries between compounds, but with low variation in measurements. The lower recoveries in VOCs can be related back to their polarity and therefore their compatibility with the desorption solvent.

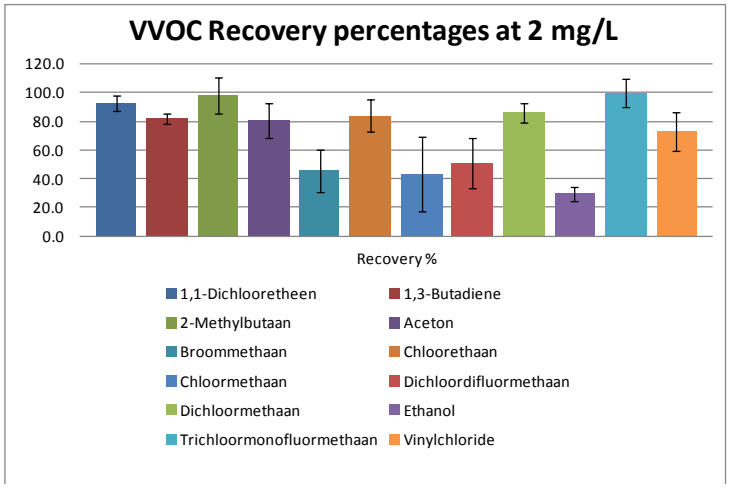

Figure 12. Very volatile organic compound recovery percentages at a spiked concentration of 2 mg/L. Chemically desorbed with carbon disulphide and analysed on GC-MS system 1. Standard deviations are included, n=3.

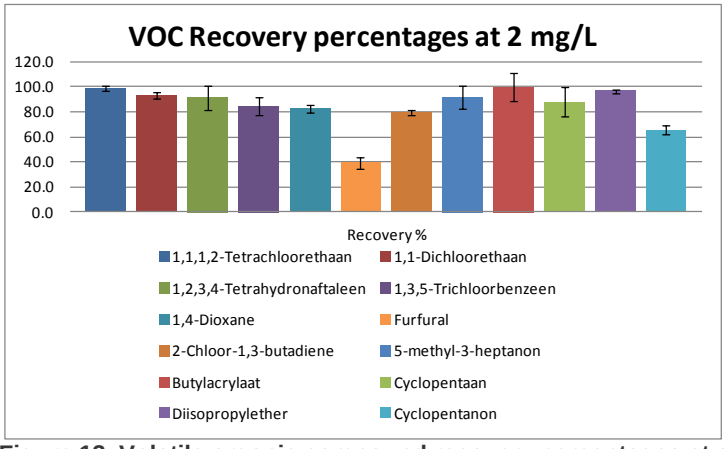

Figure 13. Volatile organic compound recovery percentages at a spiked concentration of 2 mg/L. Chemically desorbed with carbon disulphide and analysed on GC-MS system 1. Standard deviations are included, n=3.

In addition to high variation and low recoveries in VVOCs, a significant decrease in recovery occurs in the spiking level at 10 mg/L. Dichlorodifluoromethane decreased with 39.9%, trichlorofluoromethane with 38.2%, chloromethane with 13.3%, chloroethane with 45.1% and bromomethane with 18.7%. Following these results, it was first suspected that the active charcoal was perhaps saturated at this concentration and would expel the VVOCs first, before heavier compounds. This hypothesis was tested by spiking the same concentration on the badge using a standard which consisted of only 6 VVOCs. In table 4 it can be seen that this test, test 1, did not have a notable effect on the recovery percentage. Another test was performed, test 2, where the desorption was cooled by using dry ice. Since it was discovered that the desorption with carbon disulphide supposedly generated heat. Possibly causing VVOCs to evaporate rapidly during this process. Again, test results did not confirm this theory. More tests would have to be performed in order to uncover what causes this decrease in recovery at high concentration. When referring to the 3M Organic Vapour Monitor Sampling and Analysis Guide, no recovery coefficients are known for these five VVOC and a comparison cannot be made (3M Science Applied to Life, 2019).

Table 4. Test results for VVOC decrease in the 10 mg/L spiking results. Test 1: Spiking with a VVOC standard, test 2: Chilled desorption by use of dry ice. All results were measured on GC-MS system 1.

	Recovery %			
Compound	**2 mg/L**	**10 mg/L**	**test 1**	**test 2**
Dichlorodifluoromethane	50.8	10.9	10.0	15.2
Trichlorofluoromethane	99.8	61.6	73.9	67.8
Chloromethane	43.4	30.1	27.2	35.1
Chloroethane	84.2	39.1	53.1	48.8
Bromomethane	45.8	27.1	29.2	27.9

4.2 METHOD PERFORMANCE AND VALIDATION

4.2.1 LINEARITY

On GC-MS system 1, linearity was determined for all volatile organic compounds in a range of 0.1 to 10 mg/L in carbon disulphide, as was described in section 3.2.5. This range proved to be a functional working range for most compounds, with few exceptions. A linear range is approved when the correlation coefficient is equal to or exceeds the value of 0.995 and has no less than 5 data points. The following compounds measured did not meet these limitations; PGME (propylene glycol methyl ether), dimethyl formamide, 1-methyl-2-pyrrolidon, 1,3-diisopropylbenzene, n-pentane, n,n,-dimethylacetamide and ethylene glycol monobutyl ether.

Figures 14 and 15 provide some examples of acceptable and non-acceptable linearity results. Figure 14, graph number 1 is an example of an acceptable linear curve, with a correlation coefficient 0.99987, which easily surpasses the limitation value of <0.995. Curves 2 through 4 are on the other spectrum and do not pass as acceptable linear ranges. Curve number 2, while still within the acceptable range, showed a slightly curved line of data points. This occurred in more compounds, but all remained within the acceptable range.

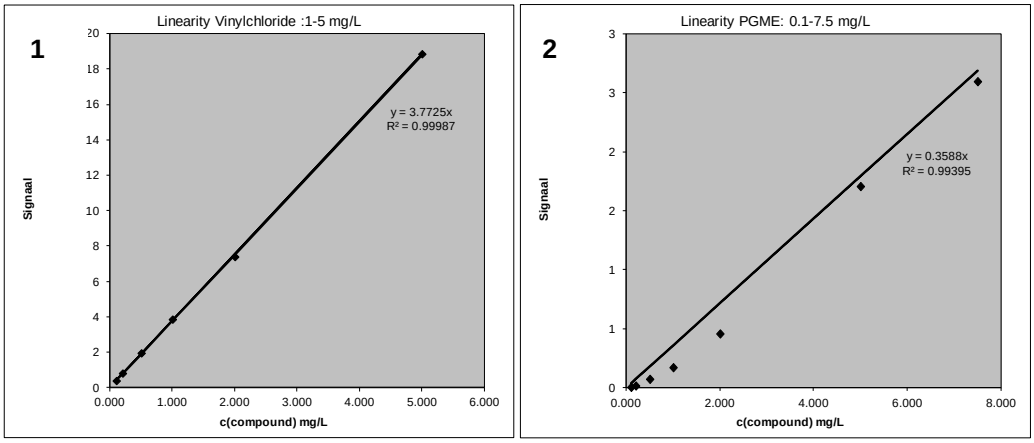

Figure 14. Examples of acceptable linear ranges, measured on GC-MS system 1.

Figure 15, on the other end of the spectrum do not pass as acceptable linear ranges. Curve number 3 demonstrated a curved line and few data points. The compound, n,n-dimethylacetamide yields a peak with low sensitivity, causing the standards of 0.1 and 0.2 to not have any area response when measured. Curve 4 belongs to the compound n-pentane and shows a constant area response, while a linear increase was expected. Reason for this is that n-pentane is the solvent for one of the internal stock solutions, causing a percentage of the desorption solvent to be pentane. Thus, the addition of any amount causes the compound to fall outside its linear range. If n-pentane would have been present in a smaller quantity, a blank correction could have been performed. The raw data and all calibration curves, for every compound measured on GC-MS system 1, can be found in Appendix IV, table 13 and figure 2.

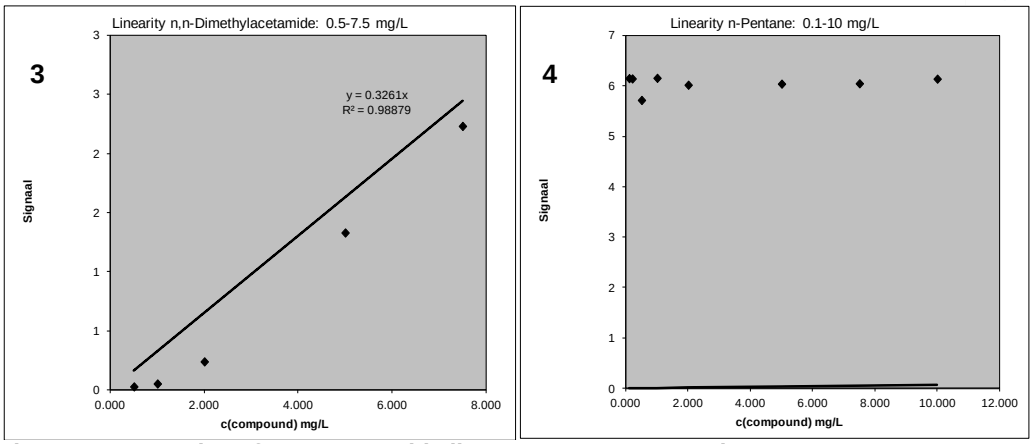

Figure 15. Examples of non-acceptable linear ranges, measured on GC-MS system 1.

4.2.2 LIMIT OF DETECTION AND QUANTITATION AND REPRODUCIBILITY

This method was validated as a manner of testing its performance and limitations for further research. The limit of detection and quantitation (LOD/LOQ) was measured to evaluate the methods sensitivity for every peak, it was attempted to measure LOD/LOQ on a spiking level of 0.1 mg/L. Many compounds showed peaks distinguishable from the noise, unfortunately a small amount did not. Such as, isophorone and diethylene glycol diethyl ether, which both have poor recovery percentages after desorption. LOD/LOQ standards as set in NEN 7777, were not met, with few exceptions, as can be seen in Appendix IV, table 14. Faulty validation results in LOD/LOQ were caused by either a lack of measurements and/or high variation in measurements.

Reproducibility validation results were inconsistent but showed promise. As can be seen in Appendix IV, tables 15 and 16, most compounds do meet the maximum variation coefficient of 20% and a number of compounds do not. The extreme cases where the variation coefficient was exceeded immensely, mostly occurred in very volatile organic compounds which yield bad desorption coefficients in desorption and thus variable results. Other compounds that do not meet the requirement often exceeded the limiting value by a small amount.

5 CONCLUSION AND RECCOMEMENDATIONS

The method which was developed for the analysis of volatile organic compounds by GC-MS and chemical desorption was developed unsuccessfully due to limitations. Low efficiency of desorption in polar compounds caused low sensitivity and unreliable results in GC-MS analysis. In addition, many compounds co-elute and interfere with results due to similarities in mass spectra. A validation was performed on GC-MS system 1 to evaluate the methods performance, but this proved to require many improvements before use in routine analysis. The secondary GC-MS system was not validated for its performance due to time limitations. It was established that the additional system could assist in the separation and detection of allyl chloride and isooctane. Further possibilities will have to be evaluated.

The following recommendations can be made to further optimize the method which was developed,

A recommendation for improved desorption efficiency would be to explore different desorption solvents or mix polar additives with carbon disulphide, which is generally used as desorption solvent. Some reports on improved desorption efficiency for polar compounds in VOC analysis include those of Diago P. Lopes, where it was found that a mixture of 4% Dimethyl sulphoxide (DMSO) in carbon disulphide (v/v), provides adequate recoveries of >75% for most glycol ether and recoveries >90% for most hydrocarbons, ketones and esters (Lopes, 1997; MDHS 88, 1997). And Steve W. Beck, who found that when using a mixture of 5% 2-2-Buthoxyethanol in carbon disulphide (v/v) significantly improved efficiency for diffusion badges and sorbent tubes (Beck, Stock, & Whitehead, 1990).

In regard to Green Analytical Chemistry and Circular Chemistry, where it is preferred to optimize recourse efficiency and minimize waste (Galuszka, Migaszewski, & Namiesnik, 2013; Keijer, Bakker, & Slootweg, 2019), another option for the process of desorption would be Thermal Desorption. This technique has advantages such as the conservation of the sample, a large dynamic range and the elimination of solvent use (Harper & Fiorito, 1996), which would be preferred for GAC purposes and analyst safety, due to the hazardous characteristics of carbon disulphide. A negative aspect of this technique in analytical application would be the fact that the sampling is performed on the sorbent tubes, not 3M badges, and that the thermal desorption system is reusable. When looking at efficiency of the desorption, chemical desorption is preferred.

A recommendation can be made to view the limit of detection and quantitation differently. Instead of viewing this parameter as the methods sensitivity per compound, look into the exposure limits at Time weight average 8 hours (t.g.g. 8h) set by the Netherlands. Volatile organic compound analysis is performed for indoor air quality and workplace safety, so it would be fit to look into these exposure limits per compound and evaluate if this concentration can be detected.

The final and perhaps most revolutionary recommendation would be to look into the application of comprehensive GC x GC hyphenated with a MS detector, which is a technique used in the SGS laboratory located in Antwerp. Cecilia Arsene stated in her review on the technique and its application for analysis of VOCs in air, that it shows great promise for VOC analysis due to its improved sensitivity, vastly increased separation space due to the added dimension and the ability to separate and identify hundreds of peaks (Arsene, Vione, Grinberg, & Olariu, 2011). Paired with different detection techniques, such as time-of-flight MS (TOF-MS), MS and FID, comprehensive GC x GC proves to be a powerful tool for various fields of research, including environmental science.

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8 APPENDIX I: COMPOUND LIST

Table 1. Complete compound list including CAS no and (recommended) desorption solvent.

No	Compound	CAS nr	Desorption solvent
1	1,1,1,2-Tetrachloroethane	630-20-6	CS_2
2	1,1,1-Trichloroethane	71-55-6	CS_2
3	1,1,2,2-Tetrachloroethane	79-34-5	CS_2
5	1,1,2-Trichloro-1,2,2-trifluoroethane	76-13-1	CS_2
4	1,1,2-Trichloroethane	79-00-5	CS_2
7	1,1-Dichloroethane	75-34-3	CS_2
8	1,1-Dichloroethene	75-35-4	CS_2
9	1,1-Dichloropropane	78-99-9	CS_2
6	1,1-Dichloropropene	563-58-6	CS_2
10	1,2,3,4-Tetrahydronaftalene	119-64-2	CS_2
11	1,2,3-Trichlorobenzene	87-61-6	CS_2
12	1,2,3-Trichloropropane	96-18-4	CS_2
13	1,2,3-Trimethylbenzene	526-73-8	CS_2
14	1,2,4-Trichlorobenzene	120-82-1	CS_2
15	1,2,4-Trimethylbenzene	95-63-6	CS_2
16	1,2-Dibromo-3-chloropropane	96-12-8	CS_2
17	1,2-Dibromoethane	106-93-4	CS_2
18	1,2-Dichlorobenzene	95-50-1	CS_2
19	1,2-Dichloroethane	107-06-2	CS_2
20	1,2-Dichloropropane	78-87-5	CS_2
21	1,2-Diethylbenzene	135-01-3	CS_2
22	1,3,5-Trichlorobenzene	108-70-3	CS_2
23	1,3,5-Trimethylbenzene	108-67-8	CS_2
24	1,3-Butadiene	106-99-0	*Methylene chloride*
25	1,3-Dichlorobenzene	541-73-1	CS_2
26	1,3-Dichloropropane	142-28-9	CS_2
27	1,3-Diethylbenzene	141-93-5	CS_2
28	1,3-Diisopropenylbenzene	3748-13-8	CS_2
29	1,4-Dichlorobenzene	106-46-7	CS_2
30	1,4-Diethylbenzene	105-05-5	CS_2
31	1,4-Diisolpropylbenzene	100-18-5	CS_2
32	1,4-Dioxane	123-91-1	CS_2
33	1-Broom-3-chloropropane	109-70-6	CS_2
34	1-Butanol	71-36-3	*Methylene chloride*
35	1-Methoxy-2-propanol acetate (PGMEA)	108-65-6	CS_2
36	1-Methyl-2-pyrrolidone	872-50-40	*Methylene chloride*
37	1-Methyl-4-isopropylbenzene	99-87-6	CS_2
38	2,2-Dichloropropane	594-20-7	CS_2
39	2,2-Dimethylbutane	75-83-2	CS_2
40	2,3-dichloropropene	78-88-6	CS_2
41	2,4-Dimethyl-3-pentanone	565-80-0	CS_2
42	2,4-Dimethylpentane	108-08-7	CS_2
43	2-Butanol	78-92-2	*Methylene chloride*
44	2-Butanone	78-93-3	CS_2
45	2-Butoxy ethyl acetate	112-07-2	CS_2
46	2-Chlorotoluene	95-49-8	CS_2
47	2-Ethoxyethanol	110-80-5	*Methylene chloride*
48	2-Ethoxyethyl acetate	111-15-9	CS_2
49	2-Ethyltoluene	611-14-3	CS_2
50	2-Methoxyethanol (methyl cellsolve)	109-86-4	*Methylene chloride*
51	2-Methyl-1-propanol	78-83-1	*Methylene chloride*
52	2-Methyl-2-butanol	75-85-4	CS_2
53	2-Methylbutane	78-78-4	CS_2
54	2-Methylcyclohexanone	583-60-8	CS_2
55	2-Methylpentane	107-83-5	CS_2

(Table 1 continuing)

No	Compound	CAS nr	Desorption solvent
56	2-Pentanol	6032-29-7	*Methylene chloride*
57	2-Propoxyethanol	2807-30-9	CS_2
58	3-Ethyltoluene	620-14-4	CS_2
59	3-Heptanone	106-35-4	CS_2
60	3-Methyl-1-butanol	123-51-3	*Methylene chloride*
61	3-Methyl-2-butanone	563-80-4	CS_2
62	3-Methylcyclohexanone	591-24-2	CS_2
63	3-Pentanol	584-02-1	CS_2
64	3-Pentanone	96-22-0	CS_2
65	4-Chlorotoluene	106-43-4	CS_2
66	4-Ethyltoluene	622-96-8	CS_2
67	4-Heptanone	123-19-3	CS_2
68	4-Hydroxy-4-methyl-2-pentanone	123-42-2	*Methylene chloride*
69	4-Methylcyclohexanone	589-92-4	CS_2
70	4-Vinyl-1-cyclohexene	100-40-3	CS_2
71	5-Methyl-3-heptanone	541-85-5	CS_2
72	Acetone	67-64-1	CS_2
73	Acrylonirtil	107-13-1	*Methylene chloride*
75	Allyl alcohol	107-18-6	*Methylene chloride*
74	Allyl chloride	107-05-1	CS_2
76	Benzene	71-43-2	CS_2
78	Benzyl acetate	140-11-4	CS_2
77	Benzyl alcohol	100-51-6	CS_2
79	Benzyl chloride	100-44-7	CS_2
81	Bromobenzene	108-86-1	CS_2
82	Bromochloromethane	74-97-5	CS_2
80	Bromomethane	74-83-9	CS_2
83	Bultylmethacrylate	97-88-1	CS_2
84	Butyl acrylate	141-32-2	CS_2
85	Butyl glycidyl ether	2426-08-6	CS_2
86	Butylbenzene	104-51-8	CS_2
87	Butylpropionate	590-01-2	CS_2
88	Chloorbenzene	108-90-7	CS_2
89	Chloroethane	75-00-3	CS_2
90	Chloromethane	74-87-3	CS_2
91	Chloroprene (2-chloro-1,3-butadiene)	126-99-8	CS_2
92	cis-1,2-Dichloroethene	156-59-2	CS_2
93	cis-1,3-Dichloropropene	10061-01-5	CS_2
94	cis-2-Methylcyclohexanol	7443-70-1	CS_2
95	cis-4-Methylcyclohexanol	7731-28-4	CS_2
96	cis-Decaline	493-01-6	CS_2
97	Cumene	98-82-8	CS_2
98	Cyclohexane	110-82-7	CS_2
99	Cyclohexanol	108-93-0	*Methylene chloride*
100	Cyclohexanone	108-94-1	CS_2
101	Cyclohexene	110-83-8	CS_2
102	Cyclopentane	287-92-3	CS_2
103	Cyclopentanone	120-92-3	CS_2
104	Decane	124-18-5	CS_2
105	Dibromochloromethane	124-48-1	CS_2

(Table 1 continuing)

No	Compound	CAS nr	Desorption solvent
106	Dibromomethane	74-95-3	CS_2
107	Dibutyl ether	142-96-1	CS_2
108	Dichlorobromomethane	75-27-4	CS_2
111	Dichlorodifluoromethane	75-71-8	CS_2
109	Dichloroethyl ether	111-44-4	CS_2
110	Dichloromethane	75-09-2	CS_2
113	Diethyl ether	60-29-7	CS_2
112	Diethylene glycol diethyl ether	112-36-7	CS_2
114	Di-iso-butyl ketone	108-83-8	CS_2
115	Di-isopropyl ether	108-20-3	CS_2
116	Dimethyl formamide	68-12-2	*Methylene chloride*
118	Dipropyleenglycol methyl ether	34590-94-8	CS_2
119	D-Limonene	5989-27-5	CS_2
120	Dodecane	112-40-3	CS_2
121	Epichlorohydrine	106-89-8	CS_2
122	Ethanol	64-17-5	CS_2
125	Ethyl acetate	141-78-6	CS_2
126	Ethyl acrylate	140-88-5	CS_2
127	Ethyl benzene	100-41-4	CS_2
123	Ethyl methacrylate	97-63-2	CS_2
124	Ethyl tert-butyl ether (ETBE)	637-92-3	CS_2
128	Ethylene chlorohydrine	107-07-3	*Methylene chloride*
130	Ethylene glycol diethyl ether	629-14-1	CS_2
131	Ethylene glycol dimethyl ether	110-71-4	CS_2
132	Ethylene glycol methylether acetate	110-49-6	CS_2
133	Ethylene glycol monobutylether	111-76-2	*Methylene chloride*
129	Ethylene glycoldiacetate	111-55-7	CS_2
134	Ethylpropionate	105-37-3	CS_2
135	Furfural	98-01-1	*Methylene chloride*
136	Furfuryl alcohol	98-00-0	*Methylene chloride*
137	Hexachlorobutadiene	87-68-3	CS_2
138	Hexachloroethane	67-72-1	CS_2
139	Hexadecane	544-76-3	CS_2
140	Iodomethane	74-88-4	CS_2
141	Isobutyl acetate	110-19-0	CS_2
142	Isobutyl benzene	538-93-2	CS_2
143	Isoforon	78-59-1	CS_2
144	isooctaan	540-84-1	CS_2
145	Isopentylacetate	123-92-2	CS_2
147	Isopropyl glycidyl ether	4016-14-2	CS_2
148	Isopropyl glycol	109-59-1	CS_2
146	Isopropylacetate	108-21-4	CS_2
149	Mesityl oxide	141-79-7	CS_2
150	Methacrylonitrile	126-98-7	CS_2
151	Methyl amyl ketone	110-43-0	CS_2
160	Methyl isoamyl ketone	110-12-3	CS_2
152	Methyl isobutyl carbinol	108-11-2	CS_2
153	Methyl isobutyl keton	108-10-1	CS_2
154	Methyl methacrylate	80-62-6	CS_2
155	Methyl propyl ketone	107-87-9	CS_2

(Table 1 continuing)

No	Compound	CAS nr	Desorption solvent
156	Methylacrylate	96-33-3	CS_2
157	Methylal	109-87-5	CS_2
158	Methylcyclohexane	108-87-2	CS_2
159	Methylcyclopentane	96-37-7	CS_2
161	Methyl-n-butyl ketone	591-78-6	CS_2
203	m-Xylene + p-Xylene	108-38-3/106-42-3	CS_2
117	N,N-Dimethylacetamide	127-19-5	*Methylene chloride*
163	n-Amyl acetate	628-63-7	CS_2
162	Naphthalene	91-20-3	CS_2
164	n-Butyl acetate	123-86-4	CS_2
165	n-Heptane	142-82-5	CS_2
166	n-Hexane	110-54-3	CS_2
167	n-Octane	111-65-9	CS_2
168	Nonane	111-84-2	CS_2
169	n-Pentane	109-66-0	CS_2
170	n-Propanol	71-23-8	*Methylene chloride*
171	n-Propyl acetate	109-60-4	CS_2
172	o-Xylene	95-47-6	CS_2
173	Pentachloroethane	76-01-7	CS_2
174	Pentadecane	629-62-9	CS_2
175	Pentanol	71-41-0	*Methylene chloride*
176	Propylbenzene	103-65-1	CS_2
177	Propylene glycol monomethyl ether (PGME)	107-98-2	*Methylene chloride*
178	sec-Butylbenzene	135-98-8	CS_2
179	Styrene	100-42-5	CS_2
180	Tert-amyl methyl ether (TAME)	994-05-8	CS_2
181	Tert-Butyl alcohol	75-65-0	CS_2
183	Tert-Butyl methyl ether (MTBE)	1634-04-4	CS_2
182	Tert-butylbenzene	98-06-6	CS_2
184	Tert-Butyltoluene	98-51-1	CS_2
185	Tetrachloorethylene	127-18-4	CS_2
186	Tetrachloromethane	56-23-5	CS_2
187	Tetradecane	629-59-4	CS_2
188	Tetrahydrofuran (THF)	109-99-9	CS_2
189	Tetrahydrothiophene	110-01-0	CS_2
190	Toluene	108-88-3	CS_2
191	trans-1,2-Dichloroethene	156-60-5	CS_2
192	trans-1,3-Dichloropropene	10061-02-6	CS_2
193	trans-2-Methylcyclohexanol	7443-52-9	CS_2
194	trans-4-methylcyclohexanol	7731-29-5	CS_2
195	trans-Decaline	493-02-7	CS_2
196	Tribromomethane (Bromoform)	75-25-2	CS_2
198	Trichloroethylene	79-01-6	CS_2
197	Trichloromethane (chloroform)	67-66-3	CS_2
199	Trichloromonfluoromethane	75-69-4	CS_2
200	Tridecane	629-50-5	CS_2
201	Undecane	1120-21-4	CS_2
202	Vinyl chloride	75-01-4	CS_2
204	α-Methylstyrene	98-83-9	CS_2
205	α-Pinene	80-56-8	CS_2

9 APPENDIX II: METHODS

Table 2. GC-MS selective ion measurement (SIM) method system 1.

SIM Window	RT	Compound	Q	M1	M2
3.00-5.32	3.28	Dichlorodifluoromethane	85	87	101
	3.74	Chloromethane	50	52	49
	4	Vinyl chloride-D3	65	67	30
	4.04	Vinyl chloride	62	64	27
	4.13	1,3-Butadiene	39	54	27
	4.93	Bromomethane	94	96	93
	5.23	Chloroethane	***64***	***66***	***49***
5.32-7.00	5.45	2-Methylbutaan	***43***	***27***	***57***
	5.90	Trichloromonfluoromethane	101	103	66
	6.15	n-Pentaan	43	57	72
	6.54	Ethanol	31	45	46
	6.69	Diethylether	31	45	59
7.00-7.80	7.30	1,1-Dichlooretheen	61	96	98
	7.32	1,1,2-Trichloro-1,2,2-trifluoroethane	101	103	151
	7.39	2,2-Dimethylbutaan	43	57	71
	7.43	Methylal	45	29	75
	7.44	Acetone	43	42	58
	7.68	Iodomethane	142	127	139
7.80-8.10 (MS OFF)	-	**CS_2 (Solvent peak)**	-	-	-
8.10-9.00	8.60	Dichloormethaan	49	84	86
	8.63	2-Methylpentaan	43	27	71
	8.70	Cyclopentaan	42	55	70
	8.87	tert-Butyl Alcohol	59	57	41
	-	Allyl chloride	41	39	76
9.00-10.00	9.23	Tert-Butylmethylether (MTBE)	73	57	41
	9.25	Acrylonirtil	53	52	26
	9.26	trans-1,2-Dichlooretheen	61	96	98
	9.89	n-Hexaan	57	43	29
10.00-10.80	10.26	Allylalcohol	57	31	39
	10.31	1,1-Dichloorethaan	63	65	27
	10.36	Di-isopropylether	45	59	87
	10.41	n-Propanol	31	42	29
	10.47	Chloroprene (2-chloro-1,3-butadiene)	53	88	27
10.80-11.45	11.12	2,4-Dimethylpentaan	43	57	85
	11.17	Ethyl tert-butyl ether (ETBE)	59	87	41
	11.31	Methylcyclopentaan	56	69	84
11.45-11.90	11.60	2-Butanone	43	57	72
	11.61	cis-1,2-Dichlooretheen	61	96	98
	11.64	2,2-Dichloorpropaan	77	41	97
	11.67	Ethylacetate	43	70	88
	11.78	Methylacrylaat	55	58	85
11.90-12.55	12.01	2-Butanol	45	59	27
	12.11	Methacrylonitrile	39	67	52
	12.13	Tetrahydrofuraan (THF)	42	71	72
	12.15	Broomchloormethaan	49	128	130
	12.38	Trichloormethaan (chloroform)	83	85	47
12.55-13.15	12.70	1,1,1-Trichloorethaan	97	61	117
	12.83	Cyclohexaan	56	69	84
	13.03	Tetrachloormethaan	117	82	47
	13.09	1,1-Dichloor propeen	***75***	***39***	***112***
13.15-13.55	13.29	2-Methyl-1-propanol	43	41	74
	13.35	2-Methoxyethanol (methyl cellsolve)	45	29	76
	13.37	Ethyleenglycoldimethylether	45	60	90
	13.5	Benzene	**78**	**77**	**51**
	13.53	2-Methyl-2-butanol	***55***	***59***	***73***
13.55-13.90	13.62	Isopropylacetaat	***43***	***61***	***87***
	13.69	isooctaan	57	56	41
	13.71	1,2-Dichloorethaan	62	49	27
	13.72	Cyclohexeen	54	67	82
	13.81	Tert-amyl methyl ether (TAME)	73	74	87
13.90-14.45	14.09	n-Heptaan	43	71	100
	14.19	3-Methyl-2-butanone	43	71	86
14.45-15.00	14.71	1-Butanol	31	41	56
	14.75	Propylene Glycol Monomethyl Ether (PGME)	45	47	31
	14.80	1,1-Dichloropropane	77	41	79
	14.93	Trichloroethylene	130	95	60

(Table 2 continuing)

SIM Window	RT	Compound	Q	M1	M2
15.00-15.60	15.14	Ethylacrylaat	55	82	99
	15.34	Methyl propyl ketone	43	58	86
	15.42	Methylcyclohexaan	83	55	98
	15.54	1,2-Dichloorpropaan	***63***	***41***	***27***
	15.58	2,3-dichloropropene	***75***	***110***	***112***
	15.58	Ethylpropionaat	***29***	***57***	***102***
15.60-15.80	15.62	Methyl methacrylaat	***41***	***69***	***100***
	15.64	3-Pentanon	***57***	***86***	***87***
	15.68	1,4-Dioxaan	***28***	***58***	***88***
15.70-16.25	15.74	Dibroommethaan	***174***	***176***	***93***
	15.76	n-Propylacetaat	***43***	***61***	***73***
	15.85	Ethyleen chloorhydrine	31	44	80
	15.91	2-Pentanol	45	55	73
	15.93	3-Pentanol	59	41	31
	16.11	Dichloorbroommethaan	83	85	129
16.25-17.25	16.38	2-Ethoxyethanol	59	45	72
	16.86	Epichloorhydrine	57	59	62
	17.08	cis-1,3-dichloropropene	75	77	110
17.25-17.90	17.39	Methyl isobutyl keton	43	58	100
	17.49	3-Methyl-1-butanol	42	55	70
	17.80	Tolueen	91	92	65
17.90-18.40	18.04	n-Octaan	43	57	85
	18.06	Isobutylacetaat	43	56	73
	18.22	Methyl Isobutyl Carbinol	45	69	87
	18.31	Isopropylglycol	43	73	89
	18.36	trans-1,3-dichloropropene	***75***	***77***	***110***
18.40-19.05	18.43	Ethyl methacrylaat	***69***	***41***	***99***
	18.61	Ethyleenglycoldiethylether	59	45	74
	18.63	Pentanol	42	55	70
	18.82	1,1,2-Trichloorethaan	97	83	61
	18.94	Tetrachloorethylene	166	129	94
19.05-19.75	19.18	2,4-Dimethyl-3-pentanone	43	71	114
	19.20	1,3-Dichloorpropaan	76	41	27
	19.28	Methyl-n-butylketon	43	58	100
	19.52	n-Butylacetaat	43	56	73
	19.53	Mesityl oxide	55	83	98
	19.63	Tetrahydrothiofeen	60	45	88
	19.68	Dibroomchloormethaan	***129***	***127***	***208***
19.75-20.40	19.84	Cyclopentanon	55	41	84
	19.91	2-Propoxyethanol	43	73	86
	19.96	4-Vinyl-1-cyclohexeen	54	79	108
	19.97	1,2-Dibroomethaan	107	109	188
	20.28	Dimethyl formamide	**73**	***44***	**28**
20.40-21.45	20.68	Ethyleenglycolmethyletheracetaat	43	45	58
	21.07	Chloorbenzeen	112	77	51
	21.14	Isopropylglycidylether	43	59	101
	21.26	Dibutylether	57	41	87
	21.29	Ethylbenzeen	91	106	65
	21.33	1,1,1,2-Tetrachloorethaan	131	117	95
21.45-21.90	21.57	1-Methoxy-2-propanolacetaat (PGMEA)	43	72	87
	21.6	Xyleen (m,p-)*	91	105	106
	21.61	Furfural	39	67	96
	21.62	Nonaan	43	57	85
	21.72	Methylisoamylketon	43	58	114
	21.72	Isopentylacetaat	43	55	70
21.90-22.35	22.05	4-Heptanon	43	71	114
	22.11	4-Hydroxy-4-methyl-2-pentanone	43	59	101
	22.26	1-Broom-3-chloorpropaan	41	77	158
22.35-22.70	22.40	Butyl acrylaat	***55***	***56***	***73***
	22.43	Furfurylalcohol	53	81	98
	22.51	o-Xyleen	91	105	106
	22.56	3-Heptanon	57	85	114
	22.57	Styreen	104	78	51
	22.67	Butylpropionaat	***57***	***75***	***87***
22.70-23.15	22.78	Methyl Amyl Ketone	***43***	***58***	***114***
	22.84	2-Ethoxyethyl acetaat	43	72	87
	22.92	n-Amylacetate	43	55	70
	23.04	Tribroommethaan (Bromoform)	173	**252**	91
	23.04	Cyclohexanol	***57***	***67***	***82***
23.15-23.60	23.23	Dimethylaceetamide	***44***	***72***	***87***
	23.36	α-Pinene	93	121	136
	23.37	Ethyleenglycolmonobutylether	57	87	100
	23.39	Cumeen	105	120	77
	23.39	3-Ethyltolueen	105	120	91

(Table 2 continuing)

SIM Window	RT	Compound	Q	M1	M2
23.60-24.55	23.86	Cyclohexanone	55	69	98
	24.15	1,1,2,2-Tetrachloorethaan	83	95	131
	24.19	Broombenzeen	77	51	156
	24.33	1,2,3-Trichloorpropaan	75	97	110
	24.35	5-Methyl-3-heptanone	57	99	128
	24.40	Propylbenzeen	91	105	120
23.55-23.90	24.66	2-Chlorotoluene	91	63	126
	24.71	4-Ethyltolueen	105	91	120
	24.73	Trans-2-Methylcyclohexanol	57	96	114
	24.85	1,3,5-Trimethylbenzeen	105	91	120
	24.85	Decaan	***57***	***85***	***142***
23.90-25.05	24.92	cis-2-Methylcyclohexanol	***68***	***81***	***96***
	24.95	4-Chlorotoluene	91	126	63
	25.01	Bultylmethacrylaat	**69**	**56**	**87**
	25.02	cis-4-Methylcyclohexanol	***57***	***81***	***96***
25.05-25.45	25.1	Trans-4-methylcyclohexanol	***57***	***81***	***96***
	25.18	Di-iso-butylketon	57	85	142
	25.27	2-Methylcyclohexanone	68	55	112
	25.3	2-Ethyltolueen	105	120	91
	25.39	α-Methylstyrene	***118***	***103***	***91***
25.45-25.90	25.57	3-Methylcyclohexanone	69	56	112
	25.62	Tert-butylbenzeen	119	91	134
	25.71	Pentachloroethane	167	117	83
	25.74	Butyl glycidyl ether	57	29	73
	25.78	1,2,4-Trimethylbenzeen	105	120	91
	25.79	4-Methylcyclohexanone	55	83	112
25.90-26.35	26.05	Ethyleenglycoldiacetaat	43	86	116
	26.11	Isobutylbenzeen	91	65	134
	26.16	sec-Butylbenzeen	105	134	91
	26.25	Dichloorethylether	***93***	***95***	***63***
26.35-26.90	26.43	D-Limoneen	***68***	***93***	***136***
	26.48	1,3-Dichloorbenzeen	146	111	75
	26.56	1-Methyl-4-isopropylbenzeen	119	134	91
	26.74	1,4-Dichloorbenzeen	146	111	75
	26.78	Dipropyleenglycol methyl ether	59	73	104
	26.79	1,2,3-Trimethylbenzeen	105	120	91
26.90-27.40	27.04	Benzylchloride	91	65	126
	27.25	1,3-Diethylbenzene	***105***	***119***	***134***
27.40-28.10	27.51	1,4-Diethylbenzene	***105***	***119***	***134***
	27.56	Butylbenzeen	91	92	134
	27.60	Trans-Decaline	67	96	138
	27.62	1,2-Dichloorbenzeen	146	111	75
	27.74	1,2-Diethylbenzeen	105	119	134
	27.82	Undecaan	57	71	85
	27.91	Diethyleenglycoldiethylether	45	59	72
28.10-28.80	28.29	Hexachloroethane	117	166	201
	28.40	2-Butoxy ethyl acetaat	57	87	100
	28.41	Benzyl alcohol	79	91	108
	28.57	Tert-Butyltolueen	133	105	148
28.80-29.80	29.02	1-Methyl-2-pyrrolidon	44	73	99
	29.02	cis-Decaline	96	109	138
	29.62	1,2-Dibroom-3-chloorpropaan	157	75	39
29.80-30.90	30.02	1,3,5-Trichloorbenzeen	180	145	109
	30.59	Dodecaan	57	71	85
	30.67	1,4-Diisolpropylbenzeen	147	119	162
30.90-32.10	31.10	1,2,3,4-Tetrahydronaftaleen	104	91	132
	31.13	Isoforon	82	54	138
	31.16	Benzylacetate	108	91	150
	31.62	1,2,4-Trichloorbenzeen	180	145	109
	31.95	Hexachloorbutadieen	225	190	260
32.10-33.35	32.31	Naftaleen	128	102	64
	32.84	1,2,3-Trichloorbenzeen	180	145	109
	33.13	Tridecaan	57	71	85
33.35-41.00	33.57	1,3-Diisopropenylbenzene	158	128	143
	35.56	Tetradecaan	57	71	85
	37.82	Pentadecaan	57	71	85
	39.94	Hexadecaan	57	71	85

Table 3. SIM method parameters for system 2, part 1 (Tracefinder part 1 and 2).

SIM Window	RT (min)	Compound	Q	M1	M2
3.00-5.00	3.57	Dichlorodifluoromethane	85	87	101
	3.75	Chloromethane	50	52	15
	3.99	Vinyl chloride	62	64	27
	4.00	Vinyl chloride-D3	65	67	30
	4.46	Bromomethane	94	96	93
	4.65	Chloroethane	64	66	49
5.00-7.00	5.54	Trichloromonfluoromethane	101	103	66
	5.89	Diethylether	31	45	59
	6.24	Iodomethane	142	127	139
	6.30	1,1-Dichlooretheen	61	96	98
	6.34	Acrylonirtil	53	52	26
	6.45	Dichloormethaan	49	84	86
	6.58	Allyl chloride	41	39	76
	6.69	1,1,2-Trichloro-1,2,2-trifluoroethane	101	103	151
7.00-9.30	7.57	trans-1,2-Dichlooretheen	61	96	98
	7.78	Tert-Butylmethylether (MTBE)	73	57	41
	7.81	1,1-Dichloorethaan	63	65	27
	8.15	Methacrylonitrile	41	67	52
	8.46	Chloroprene (2-chloro-1,3-butadiene)	53	88	90
	8.80	cis-1,2-Dichlooretheen	61	96	98
	8.90	Di-isopropylether	45	59	87
	8.94	n-Hexaan	57	86	29
	9.02	Broomchloormethaan	49	128	130
	9.14	Trichloormethaan (chloroform)	83	85	47
9.30-11.20	9.54	Ethyl tert-butyl ether (ETBE)	59	87	57
	9.58	Tetrahydrofuraan (THF)	42	41	72
	10.01	1,2-Dichloorethaan	62	49	98
	10.29	1,1,1-Trichloorethaan	97	61	117
	10.8	Benzene-D6	84	54	82
	10.85	Benzene	78	77	51
	11.03	Tetrachloormethaan	117	82	121
11.20-12.80	11.40	2,2-Dichloorpropaan	77	41	97
	11.42	1,1-Dichloropropane	77	41	79
	11.48	Tert-amyl methyl ether (TAME)	73	43	87
	11.82	1,2-Dichloorpropaan	63	41	76
	11.85	Dibroommethaan	174	176	93
	11.95	1,1-Dichloor propeen	75	39	112
	11.98	2,3-dichloropropene	75	110	112
	12.09	Dichloorbroommethaan	83	85	129
	12.12	Trichloroethylene	130	95	60
	12.30	Methyl methacrylaat	41	69	100
	12.37	n-Heptaan	43	71	100
12.80-16.10	13.18	cis-1,3-dichloropropene	75	77	110
	13.83	trans-1,3-dichloropropene	75	77	110
	14.04	1,1,2-Trichloorethaan	97	83	61
	14.36	Tolueen	91	92	65
	14.41	1,3-Dichloorpropaan	76	41	27
	14.61	Ethyl methacrylaat	69	41	99
	14.96	Dibroomchloormethaan	129	48	208
	15.27	1,2-Dibroomethaan	107	27	188
	15.51	n-Octaan	43	57	85
	15.83	Tetrachloorethylene	166	129	94

(Table 3 continuing)

SIM Window	RT (min)	Compound	Q	M1	M2
16.10-18.60	16.69	1,1,1,2-Tetrachloorethaan	131	117	95
	16.73	Chloorbenzeen	112	77	51
	17.21	Ethylbenzeen	91	106	65
	17.44	Xyleen (m,p-)*	91	105	106
	17.64	Tribroommethaan (Bromoform)	173	174	91
	17.96	o-Xyleen-D10	98	116	114
	18.00	Styreen	104	78	51
	18.12	o-Xyleen	91	105	106
	18.15	1,1,2,2-Tetrachloorethaan	83	85	131
	18.32	Nonaan	43	57	85
	18.35	1,2,3-Trichloorpropaan	75	97	110
18.60-22.00	18.94	Cumeen	105	120	77
	19.14	Broombenzeen	77	51	156
	19.71	2-Chlorotoluene	91	63	126
	19.73	Propylbenzeen	91	105	120
	19.82	4-Chlorotoluene	91	126	63
	19.94	3-Ethyltolueen	105	120	91
	19.96	4-Ethyltolueen	105	91	120
	20.08	1,3,5-Trimethylbenzeen	105	91	120
	20.29	Pentachloroethane	167	117	83
	20.39	2-Ethyltolueen	105	120	91
	20.43	1,2,4-Trimethylbenzeen	105	120	91
	20.73	Tert-butylbenzeen	119	91	134
	20.84	Decaan	57	85	142
	21.08	1,3-Dichloorbenzeen	146	111	75
	21.20	1,4-Dichloorbenzeen	146	111	75
	21.23	sec-Butylbenzeen	105	134	91
	21.47	1-Methyl-4-isopropylbenzeen	119	134	91
	21.51	1,2,3-Trimethylbenzeen	105	120	91
	21.81	1,2-Dichloorbenzeen	146	111	75
22.00-28.00	22.23	Butylbenzeen	91	92	134
	22.61	1,2-Dibroom-3-chloorpropaan	157	75	39
	23.02	Hexachloroethane	117	166	201
	24.21	1,3,5-Trichloorbenzeen	180	145	109
	25.16	1,2,4-Trichloorbenzeen	180	145	109
	25.34	Naftaleen-D8	136	108	78
	25.37	Naftaleen	128	102	64
	25.95	1,2,3-Trichloorbenzeen	180	145	109
	26.10	Hexachloorbutadieen	225	190	260

Table 4. SIM method parameters for system 2, part 2 (Tracefinder part 3 and 4).

SIM Window	RT (min)	Compound	Q	M1	M2
3.00-6.80	4.00	Vinyl chloride-D3	65	67	30
	5.30	Acetone	43	42	58
	5.34	2-Methylbutaan	43	27	72
	5.90	n-Pentaan	43	57	72
	6.19	Ethanol	31	45	46
	6.19	Methylal	45	29	75
	6.24	tert-Butyl Alcohol	59	57	41
6.80-8.75	7.20	n-Propanol	31	42	59
	7.83	Cyclopentaan	42	55	70
	7.91	2-Methylpentaan	43	42	71
	-	Allyl alcohol	57	39	31
	8.18	2-Butanone	43	57	72
	8.57	2-Butanol	45	59	27
8.75-10.15	8.94	2,2-Dimethylbutaan	43	57	71
	8.97	Ethylacetate	61	70	88
	8.97	Methylacrylaat	55	58	85
	9.49	2-Methyl-1-propanol	55	74	56
	9.53	2-Methoxyethanol (methyl cellsolve)	45	29	76
	9.89	2-Methyl-2-butanol	55	59	73
	9.96	Methylcyclopentaan	56	69	84
	9.98	2,4-Dimethylpentaan	43	57	85
10.15-10.90	10.32	Ethyleenglycoldimethylether	45	60	90
	10.35	Ethyleen chloorhydrine	31	43	49
	10.39	3-Methyl-2-butanone	43	71	86
	10.63	Isopropylacetaat	43	61	87
	10.68	1-Butanol	31	41	56
	10.8	Benzene-D6	84	54	82
10.90-12.70	11.02	Propylene Glycol Monomethyl Ether (PGME)	45	74	31
	11.15	Cyclohexaan	56	69	84
	11.28	Methyl propyl ketone	43	58	86
	11.63	3-Pentanon	57	86	29
	11.70	Cyclohexeen	54	67	82
	11.73	Ethylacrylaat	55	56	99
	11.88	2-Pentanol	45	55	73
	11.91	3-Pentanol	59	41	31
	12.04	isooctaan	57	56	41
	12.07	1,4-Dioxaan	28	58	88
	12.21	2-Ethoxyethanol	59	60	72
	12.22	Ethylpropionaat	29	57	102
	12.24	Epichloorhydrine	57	49	62
	12.29	n-Propylacetaat	43	61	73
12.70-14.75	13.05	3-Methyl-1-butanol	42	55	70
	13.11	Methyl isobutyl keton	43	58	100
	13.24	Methylcyclohexaan	83	55	98
	13.84	Dimethyl formamide	73	44	28
	13.85	Methyl Isobutyl Carbinol	45	69	87
	13.94	Isopropylglycol	43	73	89
	14.06	Pentanol	42	55	70
	14.23	Isobutylacetaat	43	56	73
	14.50	Cyclopentanon	55	41	84
	14.61	Methyl-n-butylketon	43	58	100
14.75-16.20	14.94	Mesityl oxide	55	83	98
	14.96	2,4-Dimethyl-3-pentanone	43	71	114
	14.96	Ethyleenglycoldiethylether	59	108	74
	15.22	2-Propoxyethanol	43	73	86
	15.40	n-Butylacetaat	43	56	73
	15.48	Tetrahydrothiofeen	60	45	88
	15.77	Furfural	39	67	96
	15.80	Ethyleenglycolmethyletheracetaat	43	45	58
	16.03	4-Hydroxy-4-methyl-2-pentanone	43	59	101

(Table 4 continuing)

SIM Window	RT (min)	Compound	Q	M1	M2
16.20-17.00	16.44	Isopropylglycidylether	43	59	101
	16.49	Furfurylalcohol	53	81	98
	16.56	Dimethylaceetamide	44	72	87
	16.58	4-Vinyl-1-cyclohexeen	54	79	108
	16.66	Methylisoamylketon	43	58	114
	16.77	1-Methoxy-2-propanolacetaat (PGMEA)	43	72	87
	16.86	1-Broom-3-chloorpropaan	41	77	158
17.00-18.60	17.13	4-Heptanon	43	71	114
	17.21	Isopentylacetaat	43	55	70
	17.49	3-Heptanon	57	85	114
	17.56	Methyl Amyl Ketone	43	58	114
	17.65	Cyclohexanol	57	67	82
	17.66	Dibutylether	57	41	87
	17.70	Cyclohexanone	55	69	98
	17.71	Butyl acrylaat	55	56	73
	17.73	2-Ethoxyethyl acetaat	43	72	87
	17.96	o-Xyleen-D10	98	116	114
	18.06	Butylpropionaat	57	75	87
	18.08	Ethyleenglycolmonobutylether	57	87	100
	18.18	n-Amylacetate	43	55	70
18.60-19.65	19.06	5-Methyl-3-heptanone	57	99	128
	19.11	Trans-2-Methylcyclohexanol	57	96	114
	19.27	2-Methylcyclohexanone	68	55	112
	19.30	3-Methylcyclohexanone	69	56	112
	19.33	Trans-4-methylcyclohexanol	57	81	96
	19.35	cis-4-Methylcyclohexanol	57	81	96
	19.36	cis-2-Methylcyclohexanol	57	81	96
	19.46	4-Methylcyclohexanone	55	83	112
	19.52	α-Pinene	93	121	136
19.65-20.85	19.77	Ethyleenglycoldiacetaat	43	86	116
	19.85	Di-iso-butylketon	57	85	142
	19.89	Dichloorethylether	93	95	63
	19.95	Bultylmethacrylaat	69	56	87
	20.19	Butyl glycidyl ether	57	41	55
	20.35	Dipropyleenglycol methyl ether	59	73	103
	20.36	α-Methylstyrene	118	103	91
20.85-22.90	21.04	Benzylchloride	91	65	126
	21.12	1-Methyl-2-pyrrolidon	44	42	99
	21.13	Isobutylbenzeen	91	65	134
	21.32	Benzyl alcohol	79	91	108
	21.72	D-Limoneen	68	93	136
	22.05	1,3-Diethylbenzene	105	119	134
	22.09	Diethyleenglycoldiethylether	45	59	72
	22.23	1,4-Diethylbenzene	105	109	134
	22.30	2-Butoxy ethyl acetaat	57	87	100
	22.38	1,2-Diethylbenzeen	105	119	134
	22.72	Trans-Decaline	67	96	138
22.90-24.00	23.08	Tert-Butyltolueen	133	105	148
	23.14	Undecaan	57	71	85
	23.53	Isoforon	82	54	138
	23.80	cis-Decaline	96	109	138
24.00-26.00	24.21	Benzylacetate	108	91	150
	24.77	Dodecaan	57	71	85
	24.81	1,4-Diisolpropylbenzeen	147	119	162
	24.87	1,2,3,4-Tetrahydronaftaleen	104	91	132
	25.34	Naftaleen-D8	136	108	78
26.00-35.00	26.89	1,3-Diisopropenylbenzene	158	128	143
	27.27	Tridecaan	57	71	85
	29.15	Tetradecaan	57	71	85
	30.90	Pentadecaan	57	71	85
	32.54	Hexadecaan	57	71	85

Table 5. Content of Ampoules used in the calibration standard.

Ampoule code	Concentration (mg/L)	Compounds
n.a.	1000	1,3-Butadiene
R-683 (Chem lab)	2000	1,2-Diethylbenzene
		1,3-Diethylbenzene
		1,4-Diethylbenzene
R-838 (Accu stdandard)	2000	Benzene
		Bromobenzene
		Bromochloromethane
		Bromodichloromethane
		Bromoform
		n-Butylbenzene
		sec-Butylbenzene
		tert-Butylbenzene
		Tetrachloromethane
		Chlorobenzene
		Chloroform
		2-Chlorotoluene
		4-Chlorotoluene
		Dibromochloromethane
		1,2-Dibromo-3-chloromethane
		1,2-Dibromoethane
		Dibromomethane
		1,2-Dichlorobenzene
		1,3-Dichlorobenzene
		1,4-Dichlorobenzene
		1,1-Dichloroethane
		1,2-Dichloroethane
		1,1-Dichloroethene
		cis-1,2-Dichloroethene
		trans-1,2-Dichloroethene
		1,2-Dichloropropane
		1,3-Dichloropropane
		2,2-Dichloropropane
		1,1-Dichloropropene
		cis-1,3-Dichloropropene
		trans-1,3-Dichloropropene
		Ethylbenzene
		Hexachlorobutadiene
		Cumene
		p-Isopropyltoluene
		Dichloromethane
		Naphthalene
		Propylbenzene
		Styrene
		1,1,1,2-Tetrachloroethane
		1,1,2,2-Tetrachloroethane
		Tetrachloroethene
		Toluene
		1,2,3-Trichlorobenzene
		1,2,4-Trichlorobenzene
		1,1,1-Trichloroethane
		1,1,2-Trichloroethane
		Trichloroethene
		1,2,3-Trichloropropane
		1,2,4-Trimethylbenzene
		1,3,5-Trimethylbenzene
		o-Xylene
		m-Xylene
		p-Xylene
		Bromomethane
		Chloroethane
		Chloromethane
		Dichlorodifluoromethane
		Trichlorofluoromethane
		Vinylchloride

(Table 5 continuing)

Ampoule code	Concentration (mg/L)	Compounds
R-840 (Restek)	2000	Diethylether
		Iodomethane
		Carbon disulfide
		MTBE
		Hexane
		Diisopropylether
		ETBE
		Methacrylonitril
		Tetrahydrofuran
		TAME
		Heptane
		Methylmethacrylate
		Octane
		Ethylmethacrylate
		Nonane
		Decane
R-841 (Restek)	2000	1,1,2-Trichlorotrifluoroethane
		Allylchloride
		Chloroprene
		1,1-Dichloropropane
		2,3-Dichloropropene
		3-Ethyltoluene
		4-Ethyltoluene
		2-Ethyltoluene
		Pentachloroethane
		1,2,3-Trimethylbenzene
		Hexachloroethane
		1,3,5-Trimethylbenzene

Table 6. Stock standards 1 through 7: composition and compound concentrations based on density.

Stock standard	Compound	Density	c(stock) mg/L
Stock-std-vlu-1	Ethanol	0.789	1973
	Tert-Butyl alcohol	0.781	1953
	n-Propanol	0.803	2008
	2-Butanol	0.806	2015
	2-Methyl-1-propanol	0.802	2005
	2-Methoxyethanol (methyl cellsolve)	0.965	2413
	2-Methyl-2-butanol	0.815	2038
	1-Butanol	0.810	2025
	2-Pentanol	0.812	2030
	3-Pentanol	0.815	2038
	2-Ethoxyethanol	0.930	2325
	3-Methyl-1-butanol	0.810	2025
	Methyl isobutyl carbinol	0.808	2020
	Isopropyl glycol	0.903	2258
	Pentanol	0.814	2035
	2-Propoxyethanol	0.911	2278
	4-Hydroxy-4-methyl-2-pentanone	0.931	2328
	Furfuryl alcohol	1.130	2825
	trans-2-Methylcyclohexanol	0.924	2310
	Benzyl alcohol	1.040	2600
	Allyl alcohol	0.854	2135
	Cyclohexanol	0.962	2405
	trans-4-methylcyclohexanol	0.914	2285
	cis-4-Methylcyclohexanol	0.917	2293
	cis-2-Methylcyclohexanol	0.936	2340
Stock-std-vlu-2	Acetone	0.784	1960
	2-Butanone	0.805	2013
	3-Methyl-2-butanone	0.805	2013
	Methyl propyl ketone	0.809	2023
	3-Pentanone	0.815	2038
	Methyl isobutyl keton	0.802	2005
	Methyl-n-butyl ketone	0.881	2203
	Mesityl oxide	0.858	2145
	2,4-Dimethyl-3-pentanone	0.806	2015
	Furfural	1.160	2900
	Methyl isoamyl ketone	0.802	2005
	4-Heptanone	0.820	2050
	3-Heptanone	0.812	2030
	Methyl amyl ketone	0.800	2000
	Di-iso-butyl ketone	0.802	2005
	5-Methyl-3-heptanone	0.823	2058
Stock-std-vlu-3	2-Methylbutane	0.616	1540
	n-Pentane	0.626	1565
	2-Methylpentane	0.653	1633
	2,2-Dimethylbutane	0.791	1978
	2,4-Dimethylpentane	0.697	1743
	isooctaan	0.690	1725
	Undecane	0.740	1850
	Dodecane	0.750	1875
	Tridecane	0.756	1890
	Tetradecane	0.764	1910
	Pentadecane	0.769	1923
	Hexadecane	0.773	1933
Stock-std-vlu-4	Ethyl acetate	0.902	2255
	Methyl acrylate	0.950	2375
	Isopropylacetate	0.870	2175
	Ethyl acrylate	0.940	2350
	Ethylpropionate	0.884	2210
	n-Propyl acetate	0.888	2220
	Isobutyl acetate	0.875	2188
	n-Butyl acetate	0.882	2205
	Ethylene glycol methylether acetate	1.010	2525
	N,N-Dimethylacetamide	0.940	2350
	1-Methoxy-2-propanol acetate (PGMEA)	0.970	2425
	Isopentylacetate	0.876	2190
	Butyl acrylate	0.894	2235
	2-Ethoxyethyl acetate	0.973	2433
	Butylpropionate	0.875	2188
	n-Amyl acetate	0.876	2190
	Ethylene glycoldiacetate	1.100	2750
	Bultylmethacrylate	0.894	2235
	2-Butoxy ethyl acetate	0.940	2350
	Isoforon	0.920	2300
	Benzyl acetate	1.050	2625

(Table 6 continuing)

Stock standard	Compound	Density	c(stock) mg/L
Stock-std-vlu-5	Cyclopentane	0.751	1878
	Methylcyclopentane	0.749	1873
	Cyclohexane	0.779	1948
	Cyclohexene	0.811	2028
	1,4-Dioxane	1.034	2585
	Methylcyclohexane	0.770	1925
	Cyclopentanone	0.950	2375
	Tetrahydrothiophene	0.999	2498
	4-Vinyl-1-cyclohexene	0.830	2075
	Cyclohexanone	0.948	2370
	2-Methylcyclohexanone	0.924	2310
	3-Methylcyclohexanone	0.914	2285
	4-Methylcyclohexanone	0.914	2285
	α-Pinene	0.858	2145
	α-Methylstyrene	0.910	2275
	Isobutyl benzene	0.853	2133
	D-Limonene	0.840	2100
	trans-Decaline	0.896	2240
	Tert-Butyltoluene	0.858	2145
	cis-Decaline	0.896	2240
	1,4-Diisolpropylbenzene	0.857	2143
	1,2,3,4-Tetrahydronaftalene	0.970	2425
	1,3-Diisopropenylbenzene	0.925	2313
	Ethylene chlorohydrine	1.200	3000
	Epichlorohydrine	1.181	2953
	1-Broom-3-chloropropane	1.592	3980
Stock-std-vlu-6	Dichloroethyl ether	1.220	3050
	Benzyl chloride	1.100	2750
	Methylal	0.860	2150
	Ethylene glycol dimethyl ether	0.868	2170
	Propylene glycol monomethyl ether (PGME)	0.920	2300
Stock-std-vlu-7	Dimethyl formamide	0.944	2360
	Ethylene glycol diethyl ether	0.840	2100
	Isopropyl glycidyl ether	0.924	2310
	Dibutyl ether	0.770	1925
	Ethylene glycol monobutylether	0.900	2250
	Butyl glycidyl ether	0.910	2275
	Dipropyleenglycol methyl ether	0.920	2300
	1-Methyl-2-pyrrolidone	1.030	2575
	Diethylene glycol diethyl ether	0.909	2273
	Acrylonirtil	0.810	2025

Table 7. Preparation schematic for the calibration standard (100 mg/l).

Cal standard	c (mg/L)	Stock	c(stock) mg/L	V(stock) uL	Solvent	Volume (ml)
c-vlu-lucht-gcms-G	100	Stock-std-vlu-1	2000	500	MeOH	10
		Stock-std-vlu-2	2000	500		
		Stock-std-vlu-3	2000	500		
		Stock-std-vlu-4	2000	500		
		Stock-std-vlu-5	2000	500		
		Stock-std-vlu-6	2000	500		
		Stock-std-vlu-7	2000	500		
		R-683	2000	500		
		R-838	2000	500		
		R-840	2000	500		
		R-841	2000	500		
		1,3-Butadiene	1000	1000		

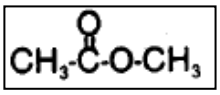
Example calculation: Diffusion coefficient (D_g)

Example calculation of the diffusion coefficient (D_g), of which the sampling rate can be derived by use of section 2.2, figures 2 through 4. This example calculation is retrieved from the 3M Sampling rate Validation protocol.

Data

Compound of interest: Methyl acetate ($C_3H_6O_2$)

Structural formula:



(3M, 1994)

MW: 74 g/mol

Boiling point: 331 ˚K

Calculation

$$\frac{kT}{\varepsilon_{12}} = \frac{28.2}{\sqrt{331}} = 1.55$$

The sampling rate validation protocol provides with a data table, to connect the found value of 1.55 with its corresponding I_d value, view Appendix II, table 8.

$$I_d = 0.5914$$

$$V_2 = \sum Atomic\ values = (3 \cdot 14.8) + (6 \cdot 3.7) + 7.4 + 9.1 = 83.1$$

To explain, 3 times 14.8 for the carbon atoms, 6 times 3.7 for the hydrogen atoms, 7.4 for the doubly bound oxygen and 9.1 for the oxygen atom inside the carbon chain, see table 1 (2.2).

$$\sqrt[3]{V_2} = \sqrt[3]{83.1} = 4.36$$

$$D_g = \frac{\left(22.03 - 5.07\sqrt{0.0345 + \frac{1}{M_1}}\right)\left(\sqrt{0.0345 + \frac{1}{M_2}}\right)}{I_d(3.62 + 1.18\sqrt[3]{V_2})^2}$$

$$D_g = \frac{\left(22.03 - 5.07\sqrt{0.0345 + \frac{1}{74}}\right)\left(\sqrt{0.0345 + \frac{1}{74}}\right)}{0.5914(3.62 + 1.18\sqrt[3]{4.33})^2} = 0.1009\ cm^2/sec$$

Table 8. Interpolated values of collision integral (3M, 1994)**.**

kT/ε_{12}	I_d	kT/ε_{12}	I_d
1.00	0.7197	**1.40**	0.6166
1.01	0.7165	1.41	0.6148
1.02	0.7132	1.42	0.6131
1.03	0.7100	1.43	0.6114
1.04	0.7067	1.44	0.6096
1.05	0.7035	1.45	0.6078
1.06	0.7003	1.46	0.6061
1.07	0.6070	1.47	0.6044
1.08	0.6938	1.48	0.6026
1.09	0.6905	1.49	0.6008
1.10	0.6873	**1.50**	0.5991
1.11	0.6846	1.51	0.5976
1.12	0.6819	1.52	0.5960
1.13	0.6791	1.53	0.5945
1.14	0.6764	1.54	0.5929
1.15	0.6737	1.55	0.5914
1.16	0.671	1.56	0.5899
1.17	0.6683	1.57	0.5883
1.18	0.6655	1.58	0.5868
1.19	0.6628	1.59	0.5852
1.20	0.6601	**1.60**	0.5837
1.21	0.6578	1.61	0.5823
1.22	0.6554	1.62	0.5810
1.23	0.6531	1.63	0.5796
1.24	0.6507	1.64	0.5783
1.25	0.6484	1.65	0.5769
1.26	0.6461	1.66	0.5755
1.27	0.6437	1.67	0.5742
1.28	0.6414	1.68	0.5728
1.29	0.6390	1.69	0.5715
1.30	0.6367	**1.70**	0.5701
1.31	0.6347	1.71	0.5689
1.32	0.6327	1.72	0.5677
1.33	0.6307	1.73	0.5665
1.34	0.6287	1.74	0.5653
1.35	0.6266	1.75	0.5640
1.36	0.6246	1.76	0.5628
1.37	0.6226	1.77	0.5616
1.38	0.6206	1.78	0.5604
1.39	0.6186	1.79	0.5592
1.40	0.6166	**1.80**	0.5580

Table 9. Diffusion coefficients and sampling rate for compound several compound classes, retrieved from the '3M Sampling rate validation protocol' (3M, 1994)

Classes	Compounds	Hirschfelder diffusion coefficient (cm^2/sec)	Mesured sampling rate (cc/min)	SD
Ketones	Acetone	0.1096	40.01	0.9
	Diisobutyl ketone	0.0606	24.6	0.8
	Methyl butyl ketone	0.0756	29.7	0.7
	Methyl isobutyl ketone	0.0761	30.0	0.4
	Methyl ethyl ketone	0.0943	36.3	0.9
	Methyl propyl ketone	0.0838	33.0	0.5
Alcohols	n-Amyl alcohol	0.0787	31.2	0.4
	iso Amyl alcohol	0.0790	32.3	0.4
	Butyl alcohol	0.0873	34.3	0.7
	Diacetone alcohol	0.0707	28.2	0.4
	iso Butyl alcohol	0.0878	35.9	0.7
	Propyl alcohol	0.1004	39.7	0.7
Aliphatics	Pentane	0.0892	34.5	0.8
	Hexane	0.0796	32.0	0.7
	Heptane	0.0721	28.9	0.7
	Octane	0.0664	26.6	0.6
	Nonane	0.0617	24.6	0.6
Cellosolve	Butyl cellosolve	0.0677	28.2	0.6
	Cellosolve	0.0815	32.4	0.9
	Cellosolve acetate	0.0682	26.6	0.4
	Methyl cellosolve	0.0911	36.6	0.4
	Methyl cellosolve acetate	0.0740	29.0	0.5
Esters	n-Amyl acetate	0.0668	26.0	0.5
	sec-Butyl acetate	0.0728	28.6	0.4
	Ethyl acetate	0.0883	34.5	0.6
	iso Butyl acetate	0.0724	31.0	0.3
	Methyl acetate	0.1009	37.0	0.6
	Propyl acetate	0.0793	30.1	0.5
Aromatics	Benzene	0.0934	35.5	0.6
	para-tert-Butyl toluene	0.0599	20.7	0.4
	Cumene	0.0690	24.5	0.9
	Mesitylene	0.0685	26.3	0.7
	Alpha methyl styrene	0.0700	25.0	0.5
	Styrene	0.0764	26.8	0.8
	Toluene	0.0827	31.4	0.6
	Xylene	0.0748	27.3	0.5
	Cyclohexanone	0.0802	28.9	0.3
	Isophorone	0.0635	21.7	0.7
	Cyclohexane	0.0851	32.4	0.7
	Cyclohexene	0.0876	32.3	0.4
	Methyl cyclohexane	0.0769	28.9	0.4
	Cyclohexanol	0.0767	29.5	0.3
Halogenated	Carbon tetrachloride	0.0857	30.2	0.4
	Chlorobenzene	0.0805	29.3	0.6
	Chlorobromomethane	0.1005	34.4	0.9
	ortho-Dichlorobenzene	0.0718	27.8	0.6
	1,2-Dichloroethylene	0.0992	35.2	0.5
	Ethyl bromide	0.1017	36.4	0.3
	Ethylene dibromide	0.0824	29.6	0.4
	Ethylene dichloride	0.0942	33.2	0.7
	Methyl chloroform	0.0855	30.9	0.3
	Methylene chloride	0.1102	37.9	0.3
	Perchloroethylene	0.0786	28.3	0.5
	Propylene dichloride	0.0833	30.6	0.4
	1,1,2-Trichloroethane	0.0836	29.7	0.6
	Trichloroethylene	0.0874	31.1	0.2

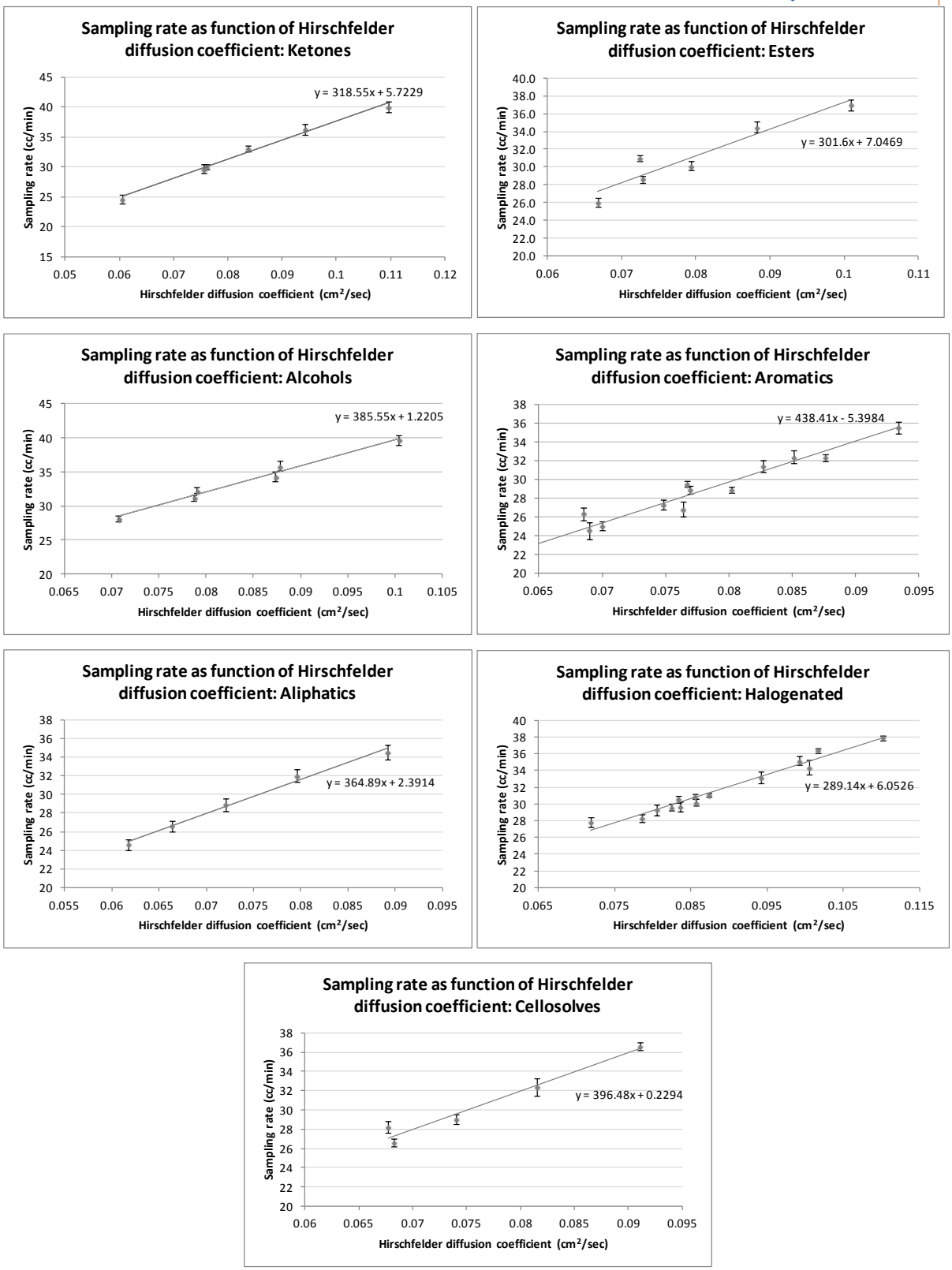


Figure 1. Sampling rate curves for compound classes; ketones, esters, alcohols, aromatics, aliphatics, halogenated compounds and cellosolves. Derived from the raw data presented in table 5 (Appendix II). Including standard deviation and the function of the line.

Table 10. Sampling rates, both theoretically calculated and provided by 3M, for all volatile organic compounds.

Compound	MW	T_b (°K)	KT/ε_{12}	I_d	V_2	$^3V\,V_2$	D_g	Category	Sampling rate cc/min
1,1,1,2-Tetrachloroethane	-	-	-	-	-	-	-		28.4[a]
1,1,1-Trichloroethane	-	-	-	-	-	-	-		30.9[a]
1,1,2,2-Tetrachloroethane	167.85	419.8	1.38	0.6206	123.4	4.978575	0.0755	Halogenated	27.9[b]
1,1,2-Trichloro-1,2,2-trifluoroethane	-	-	-	-	-	-	-		29.1[a]
1,1,2-Trichloroethane	-	-	-	-	-	-	-		29.7[a]
1,1-Dichloro-1-propene	110.97	349.7	1.51	0.5976	102.4	4.678428	0.0876	Halogenated	31.4[b]
1,1-Dichloroethane	-	-	-	-	-	-	-		33.2[a]
1,1-Dichloroethene	-	-	-	-	-	-	-		35.1[a]
1,1-Dichloropropane	112.99	361.15	1.48	0.6026	109.8	4.788514	0.0843	Halogenated	30.4[b]
1,2,3,4-Tetrahydronaftalene	132.21	480.2	1.29	0.639	162.4	5.455845	0.0666	Aromatics	23.8[b]
1,2,3-Trichlorobenzene	181.45	484.2	1.28	0.6414	149.7	5.309748	0.0671	Halogenated	25.4[b]
1,2,3-Trichloropropane	-	-	-	-	-	-	-		27.4[a]
1,2,3-Trimethylbenzene	120.19	449.2	1.33	0.6307	162.6	5.458084	0.0680	Aromatics	24.4[b]
1,2,4-Trichlorobenzene	181.45	487.55	1.28	0.6414	149.7	5.309748	0.0671	Aromatics	24.0[b]
1,2,4-Trimethylbenzene	120.19	442.2	1.34	0.6287	162.6	5.458084	0.0682	Aromatics	24.5[b]
1,2-Dibromo-3-chloropropane	236.33	471.2	1.30	0.6367	96.5	4.586793	0.0797	Halogenated	29.1[b]
1,2-Dibromoethane	-	-	-	-	-	-	-		29.6[a]
1,2-Dichlorobenzene	-	-	-	-	-	-	-		27.8[a]
1,2-Dichloroethane	-	-	-	-	-	-	-		33.2[a]
1,2-Dichloropropane	-	-	-	-	-	-	-		30.6[a]
1,2-Diethylbenzene	134.22	457.2	1.32	0.6327	169.8	5.537485	0.0659	Aromatics	23.5[b]
1,3,5-Trichlorobenzene	181.45	481.2	1.29	0.639	149.7	5.309748	0.0673	Aromatics	24.1[b]
1,3,5-Trimethylbenzene	-	-	-	-	-	-	-		26.3[a]
1,3-Butadiene	-	-	-	-	-	-	-		42.8[a]
1,3-Dichlorobenzene	147.00	446.15	1.34	0.6287	131.8	5.089071	0.0733	Halogenated	27.2[b]
1,3-Dichloropropane	112.99	393.2	1.42	0.6131	109.8	4.788514	0.0829	Halogenated	30.0[b]
1,3-Diethylbenzene	134.22	454.85	1.32	0.6327	184.8	5.695965	0.0635	Aromatics	22.5[b]
1,3-Diisopropenylbenzene	158.24	504.2	1.26	0.6461	214.4	5.985148	0.0576	Aromatics	19.8[b]
1,4-Dichlorobenzene	-	-	-	-	-	-	-		27.8[a]
1,4-Diethylbenzene	134.22	411.55	1.39	0.6186	184.8	5.695965	0.0650	Aromatics	23.1[b]
1,4-Diisopropylbenzene	162.27	483.2	1.28	0.6414	229.2	6.119814	0.0562	Aromatics	19.2[b]
1,4-Dioxane	-	-	-	-	-	-	-		34.5[a]
1-Bromo-3-chloropropane	157.44	416.4	1.38	0.6206	115.2	4.865762	0.0781	Halogenated	28.6[b]
1-Butanol	-	-	-	-	-	-	-		34.3[a]
1-Methoxy-2-propanolacetate (PGMEA)	-	-	-	-	-	-	-		25.2[a]
1-Methyl-2-pyrrolidone	-	-	-	-	-	-	-		28.8[a]
1-Methyl-4-isopropylbenzene	134.21	450.2	1.33	0.6307	184.8	5.695965	0.0637	Aromatics	22.5[b]
2,2-Dichloropropane	112.98	342.5	1.52	0.596	115.8	4.874194	0.0834	Halogenated	30.2[b]
2,2-Dimethylbutane	86.17	322.9	1.57	0.5883	140.6	5.199901	0.0803	Aliphatics	31.7[b]
2,3-Dichloropropene	110.97	367.15	1.47	0.6044	105.4	4.723677	0.0856	Halogenated	30.8[b]
2,4-Dimethyl-3-pentanone	114.19	397.2	1.41	0.6148	162.8	5.46032	0.0701	Ketones	28.0[b]
2,4-Dimethylpentane	100.20	353.5	1.50	0.5991	162.8	5.46032	0.0729	Aliphatics	29.0[b]
2-Butanol	-	-	-	-	-	-	-		34.8[a]
2-Butanone	-	-	-	-	-	-	-		36.3[a]
2-Butoxy ethyl acetate	-	-	-	-	-	-	-		24.3[a]
2-Chlorotoluene	-	-	-	-	-	-	-		27.3[a]
2-Ethoxyethanol	-	-	-	-	-	-	-		32.4[a]
2-Ethoxyethylacetate	-	-	-	-	-	-	-		26.6[a]
2-Ethyltoluene	120.19	435.0	1.35	0.6266	162.6	5.458084	0.0685	Aromatics	24.6[b]

(Table 10 continuing)

Compound	MW	T_b (°K)	KT/ε_{12}	I_d	V_2	$^3V\,V_2$	D_g	Category	Sampling rate cc/min
2-Methoxyethanol	-	-	-	-	-	-	-		36.3[a]
2-Methyl-1-propanol	-	-	-	-	-	-	-		35.9[a]
2-Methyl-2-butanol	88.15	375.0	1.46	0.6061	131.2	5.081336	0.0800	Alcohol	32.1[b]
2-Methylbutane	72.15	301.0	1.63	0.5796	118.4	4.910404	0.0895	Aliphatics	35.1[b]
2-Methylcyclohexanone	112.17	435.7	1.35	0.6266	140.4	5.197435	0.0733	Aromatics	26.7[b]
2-Methylpentane	86.18	333.2	1.54	0.5929	140.6	5.199901	0.0797	Aliphatics	31.5[b]
2-Pentanol	88.15	392.5	1.42	0.6131	131.2	5.081336	0.0791	Alcohols	31.7[b]
2-Propoxyethanol	104.15	423.0	1.37	0.6226	142.2	5.219552	0.0739	Alcohol	29.7[b]
3-Ethyltoluene	120.19	434.5	1.35	0.6266	162.6	5.458084	0.0685	Aromatics	24.6[b]
3-Heptanone	-	-	-	-	-	-	-		28.0[a]
3-Methyl-1-butanol	-	-	-	-	-	-	-		32.3[a]
3-Methyl-2-butanone	-	-	-	-	-	-	-		32.8[a]
3-Methylcyclohexanone	112.17	442.7	1.34	0.6287	140.4	5.197435	0.0731	Aromatics	26.6[b]
3-Pentanol	88.15	389.4	1.43	0.6114	131.2	5.081336	0.0793	Alcohols	31.8[b]
3-Pentanon	-	-	-	-	-	-	-		32.7[a]
4-Chlorotoluene	126.58	435.2	1.35	0.6266	136.1	5.143823	0.0735	Halogenated	27.3[b]
4-Ethyltoluene	120.20	435.0	1.35	0.6266	162.6	5.458084	0.0685	Aromatics	24.6[b]
4-Heptanone	-	-	-	-	-	-	-		27.8[a]
4-Hydroxy-4-methyl-2-pentanone	-	-	-	-	-	-	-		28.2[a]
4-Methylcyclohexanone	112.17	443.2	1.34	0.6287	140.4	5.197435	0.0731	Aromatics	26.6[b]
4-Vinyl-1-cyclohexene	-	-	-	-	-	-	-		27.9[a]
5-Methyl-3-heptanone	-	-	-	-	-	-	-		26.4[a]
Acetone	-	-	-	-	-	-	-		40.1[a]
Acrylonirtil	-	-	-	-	-	-	-		43.8[a]
Allyl alcohol	-	-	-	-	-	-	-		40.4[a]
Allyl chloride	-	-	-	-	-	-	-		35.1[a]
Benzene	-	-	-	-	-	-	-		35.5[a]
Benzyl alcohol	108.14	478.2	1.29	0.6390	131	5.078753	0.0743	Aromatics	27.2[b]
Benzyl chloride	-	-	-	-	-	-	-		27.2[a]
Benzylacetate	150.18	487.2	1.28	0.6414	173.6	5.578489	0.0638	Aromatics	22.6[b]
Benzylmethylketone	134.17	489.7	1.27	0.6437	162.6	5.458084	0.0660	Aromatics	23.5[b]
Bromobenzene	157.01	429.2	1.36	0.6246	119.3	4.922815	0.0765	halogenated	28.2[b]
Bromochloromethane	129.38	341.3	1.53	0.5945	70.8	4.136926	0.1004	Halogenated	35.1[b]
Bromomethane	-	-	-	-	-	-	-		40.9[a]
Bultylmethacrylate	142.20	433.0	1.36	0.6246	188.6	5.734742	0.0635	Ketones	26.0[b]
Butyl glycidyl ether	-	-	-	-	-	-	-		27.0[a]
Butylacrylate	-	-	-	-	-	-	-		27.3[a]
Butylbenzene	134.22	456.4	1.32	0.6327	184.8	5.695965	0.0635	Aromatics	22.5[b]
Butylpropionate	130.20	419.2	1.38	0.6206	173.8	5.58063	0.0667	Ketones	27.0[b]
Chlorobenzene	-	-	-	-	-	-	-		29.3[a]
Chloroethane	64.51	285.45	1.67	0.57423	69.7	4.115389	0.1133	Aliphatics	43.7[b]
Chloromethane	50.49	248.95	1.79	0.5592	47.5	3.621578	0.1394	Aliphatics	53.3[b]
cis-1,2-Dichloroethene	-	-	-	-	-	-	-		35.2[a]
cis-1,3-dichloropropene	110.97	377.15	1.45	0.6078	102.4	4.678428	0.0861	Halogenated	31.0[b]
cis-2-Methylcyclohexanol	114.19	438.2	1.35	0.6266	153.2	5.350811	0.0706	Aromatics	25.5[b]
cis-4-Methylcyclohexanol	114.19	445.2	1.34	0.6287	153.2	5.350811	0.0703	Aromatics	25.4[b]
cis-Decaline	138.25	463.2	1.31	0.6347	184.6	5.69391	0.0632	Aromatics	22.3[b]
Cumene	-	-	-	-	-	-	-		24.5[a]
Cyclohexane	-	-	-	-	-	-	-		32.4[a]
Cyclohexanol	-	-	-	-	-	-	-		29.5[a]
Cyclohexanone	-	-	-	-	-	-	-		28.9[a]

(Table 10 continuing)

Compound	MW	T_b (°K)	KT/ε_{12}	I_d	V_2	$^3V V_2$	D_g	Category	Sampling rate cc/min
Cyclohexene	-	-	-	-	-	-	-		32.3[a]
Cyclopentane	-	-	-	-	-	-	-		36.2[a]
Cyclopentanone	84.12	404.2	1.40	0.6166	99.5	4.63384	0.0886	Aromatics	33.4[b]
Dibromochloromethane	-	-	-	-	-	-	-		34.4[a]
Dibromomethane	173.83	370.1	1.47	0.6044	76.2	4.239536	0.0938	Halogenated	33.2[b]
Dibutylether	130.23	414.0	1.39	0.6186	196.0	5.808786	0.0635	Ester (Ether)	26.2[b]
Dichlorobromomethane	163.80	363.2	1.48	0.6026	88.7	4.459723	0.0890	Halogenated	31.8[b]
Dichlorodifluoromethane	120.91	243.35	1.81	0.5592	75.4	4.224647	0.1048	Halogenated	36.4[b]
Dichloroethylether	-	-	-	-	-	-	-		26.1[a]
Dichloromethane	-	-	-	-	-	-	-		37.9[a]
Diethylene glycoldiethylether	162.22	462.2	1.31	0.6347	218.0	6.018462	0.0581	Ester (Ether)	24.6[b]
Diethylether	-	-	-	-	-	-	-		36.8[a]
Di-iso-butylketone	-	-	-	-	-	-	-		24.6[a]
Di-isopropylether	-	-	-	-	-	-	-		31.2[a]
Dimethyl formamide	-	-	-	-	-	-	-		35.5[a]
Dipropylene glycomethylether	-	-	-	-	-	-	-		25.3[a]
D-Limonene	136.23	449.2	1.33	0.6307	192.2	5.771001	0.0626	Aromatics	22.0[b]
Epichlorohydrine	-	-	-	-	-	-	-		29.6[a]
Ethanol									43.7[a]
Ethyl methacrylate	114.14	390.2	1.43	0.6114	144.2	5.243908	0.0742	Ketones	29.4[b]
Ethyl tert-butyl ether	102.17	344.2	1.52	0.5960	151.6	5.332118	0.0753	Ester (Ether)	29.8[b]
Ethylacetate	-	-	-	-	-	-	-		34.5[a]
Ethylacrylate	-	-	-	-	-	-	-		32.2[a]
Ethylbenzene	-	-	-	-	-	-	-		27.3[a]
Ethylene chlorohydrine	-	-	-	-	-	-	-		33.9[a]
Ethyleneglycoldiacetate	146.14	463.2	1.31	0.6347	158.8	5.415229	0.0671	Ketones	27.1[b]
Ethyleneglycoldiethylether	118.17	392.6	1.42	0.6131	162.6	5.458084	0.0701	Ester (Ether)	28.2[b]
Ethyleneglycoldimethylether	90.12	358.2	1.49	0.6008	116.0	4.876999	0.0847	Ester (Ether)	32.6[b]
Ethyleneglycolmethyletheracetate	-	-	-	-	-	-	-		29.0[a]
Ethyleneglycolmonobutylether	-	-	-	-	-	-	-		28.2[a]
Ethylpropionate	102.13	372.1	1.46	0.6061	129.4	5.057991	0.0792	Ketones	30.9[b]
Furfural	-	-	-	-	-	-	-		34.3[a]
Furfurylalcohol	-	-	-	-	-	-	-		30.6[a]
Hexachlorobutadiene	-	-	-	-	-	-	-		22.9[a]
Hexachloroethane	-	-	-	-	-	-	-		26.7[a]
Iodomethane	-	-	-	-	-	-	-		36.7[a]
Isobutylacetate	-	-	-	-	-	-	-		31.0[a]
Isobutylbenzene	134.22	446.2	1.34	0.6287	184.8	5.695965	0.0639	Aromatics	22.6[b]
Isooctane	114.23	372.4	1.46	0.6061	185.0	5.698019	0.0673	Aliphatics	26.9[b]
Isopentylacetate	-	-	-	-	-	-	-		27.2[a]
Isophorone	-	-	-	-	-	-	-		21.7[a]
Isopropylacetate	-	-	-	-	-	-	-		31.7[a]
Isopropylglycidylether	-	-	-	-	-	-	-		29.1[a]
Isopropylglycol	-	-	-	-	-	-	-		29.5[a]
Mesityloxide	-	-	-	-	-	-	-		31.2[a]
Methacrylonitrile	69.09	363.45	1.48	0.6026	93.3	4.535521	0.0954	Halogenated	33.6[b]
Methyl acrylate	-	-	-	-	-	-	-		35.8[a]
Methyl Amyl Ketone	-	-	-	-	-	-	-		27.9[a]
Methyl isoamyl ketone	-	-	-	-	-	-	-		28.0[a]
Methyl Isobutyl Carbinol	-	-	-	-	-	-	-		29.2[a]
Methyl isobutyl ketone	-	-	-	-	-	-	-		30.0[a]

(Table 10 continuing)

Compound	MW	T_b (°K)	KT/ε_{12}	I_d	V_2	$^3V V_2$	D_g	Category	Sampling rate cc/min
Methyl methacrylate	-	-	-	-	-	-	-		31.8[a]
Methyl propyl ketone	-	-	-	-	-	-	-		33.0[a]
Methylal	-	-	-	-	-	-	-		37.9[a]
Methylcyclohexane	-	-	-	-	-	-	-		28.9[a]
Methylcyclopentane	84.16	345.0	1.52	0.596	121.7	4.955607	0.0844	Aromatics	31.6[b]
Methyl-n-butylketone	-	-	-	-	-	-	-		29.7[a]
n,n-Dimethylacetamide	-	-	-	-	-	-	-		32.0[a]
n-Amylacetate	-	-	-	-	-	-	-		26.0[a]
Naphthalene	-	-	-	-	-	-	-		24.6[a]
n-Butylacetate	-	-	-	-	-	-	-		31.6[a]
n-Decane	-	-	-	-	-	-	-		23.1[a]
n-Dodecane	-	-	-	-	-	-	-		21.5[a]
n-Heptane	-	-	-	-	-	-	-		28.9[a]
n-Hexaan	-	-	-	-	-	-	-		32.0[a]
n-Hexadecane	226.44	560.0	1.19	0.6628	362.6	7.130871	0.0432	Aliphatic	18.2[b]
n-Nonane	-	-	-	-	-	-	-		24.6[a]
n-Octane	-	-	-	-	-	-	-		26.6[a]
n-Pentane	-	-	-	-	-	-	-		35.3[a]
n-Propanol	-	-	-	-	-	-	-		39.7[a]
n-Propylacetate	-	-	-	-	-	-	-		30.1[a]
Pentachloroethane	202.29	435.2	1.35	0.6266	141.3	5.208517	0.0699	halogenated	26.3[b]
Pentadecane	212.41	544.2	1.21	0.6578	340.4	6.982268	0.0450	Aliphatic	18.8[b]
Pentanol	-	-	-	-	-	-	-		31.2[a]
Propylbenzene	120.19	432.2	1.36	0.6246	162.6	5.458084	0.0687	Aromatics	24.7[b]
Propylene Glycol Monomethyl Ether (PGME)	-	-	-	-	-	-	-		32.4[a]
sec-Butylbenzene	134.22	446.7	1.33	0.6307	184.8	5.695965	0.0637	Aromatics	22.5[b]
Styrene	-	-	-	-	-	-	-		28.9[a]
tert-Amyl methyl ether (TAME)	102.18	359.15	1.49	0.6008	150.5	5.31919	0.0750	Ester (Ether)	29.7[b]
tert-Butyl Alcohol	-	-	-	-	-	-	-		35.2[a]
tert-Butylbenzene	134.22	442.2	1.34	0.6287	184.8	5.695965	0.0639	Aromatics	22.6[b]
tert-Butylmethylether (MTBE)	-	-	-	-	-	-	-		30.8[a]
tert-Butyltoluene	-	-	-	-	-	-	-		20.7[a]
Tetrachloroethylene	-	-	-	-	-	-	-		28.3[a]
Tetrachloromethane	-	-	-	-	-	-	-		30.2[a]
Tetradecane	198.39	526.8	1.23	0.6531	318.2	6.827055	0.0469	Aliphatics	19.5[b]
Tetrahydrofuran	-	-	-	-	-	-	-		37.2[a]
Tetrahydrothiophene	88.17	394.3	1.42	0.6131	102.9	4.686031	0.0874	Aromatics	32.9[b]
Toluene	-	-	-	-	-	-	-		31.4[a]
trans-1,2-Dichloroethene	-	-	-	-	-	-	-		35.2[a]
trans-1,3-dichloropropene	110.97	377.15	1.45	0.6078	102.4	4.678428	0.0861	Halogenated	31.0[b]
trans-2-Methylcyclohexanol	114.19	440.8	1.34	0.6287	153.2	5.350811	0.0703	Alcohol	28.3[b]
trans-4-methylcyclohexanol	114.19	445.2	1.34	0.6287	153.2	5.350811	0.0703	Alcohol	28.3[b]
trans-Decaline	138.25	458.2	1.32	0.6327	184.6	5.69391	0.0634	Aromatics	22.4[b]
Tribromomethane (Bromoform)	-	-	-	-	-	-	-		29.3[a]
Trichloroethylene	-	-	-	-	-	-	-		31.1[a]
Trichloromethane (Chloroform)	-	-	-	-	-	-	-		33.5[a]
Trichloromonofluoromethane	137.37	296.92	1.64	0.5783	88.3	4.453009	0.0942	Halogenated	33.3[b]
Tridecane	184.37	507.2	1.25	0.6484	296.0	6.664444	0.0491	Aliphatics	20.3[b]
Undecane	153.31	469.2	1.30	0.6367	251.6	6.313016	0.0545	Aliphatics	22.3[b]
Vinyl chloride	-	-	-	-	-	-	-		40.8[a]
Xylene (m,p-)	-	-	-	-	-	-	-		27.3[a]
Xylene (o)	-	-	-	-	-	-	-		27.3[a]
α-Methylstyrene	-	-	-	-	-	-	-		25.0[a]
α-Pinene	136.23	429.30	1.36	0.6246	187.2	5.720517	0.0639	Aromatics	22.6[b]

a: Sampling rate provided/determined by 3M (3M Science Applied to Life, 2019)

b: Sampling rate determined theoretically

10 APPENDIX III: RESULTS METHOD DEVELOPMENT

Table 11. Elution order and retention times in minutes of GC-MS system 2.

RT (min)	Compound
3.28	Dichlorodifluoromethane
3.74	Chloromethane
4.04	Vinyl chloride
4.13	1,3-Butadiene
4.93	Bromomethane
5.23	Chloroethane
5.45	2-Methylbutane
5.90	Trichloromonfluoromethane
6.15	n-Pentane
6.54	Ethanol
6.69	Diethyl ether
7.30	1,1-Dichloroethene
7.32	1,1,2-Trichloro-1,2,2-trifluoroethane
7.39	2,2-Dimethylbutane
7.43	Methylal
7.44	Acetone
7.68	Iodomethane
8.60	Dichloromethane
8.63	2-Methylpentane
8.70	Cyclopentane
8.87	Tert-Butyl alcohol
9.23	Tert-Butyl methyl ether (MTBE)
9.25	Acrylonirtil
9.26	trans-1,2-Dichloroethene
9.89	n-Hexane
10.26	Allyl alcohol
10.31	1,1-Dichloroethane
10.36	Di-isopropyl ether
10.41	n-Propanol
10.47	Chloroprene (2-chloro-1,3-butadiene)
11.12	2,4-Dimethylpentane
11.17	Ethyl tert-butyl ether (ETBE)
11.31	Methylcyclopentane
11.60	2-Butanone
11.61	cis-1,2-Dichloroethene
11.64	2,2-Dichloropropane
11.67	Ethyl acetate
11.78	Methyl acrylate
12.01	2-Butanol
12.11	Methacrylonitrile
12.13	Tetrahydrofuran (THF)
12.15	F75-27-4
12.38	Trichloromethane (chloroform)
12.70	1,1,1-Trichloroethane
12.83	Cyclohexane
13.03	Tetrachloromethane
13.09	1,1-Dichloropropene
13.29	2-Methyl-1-propanol
13.35	2-Methoxyethanol (methyl cellsolve)
13.37	Ethylene glycol dimethyl ether
13.50	Benzene
13.53	2-Methyl-2-butanol
13.62	Isopropylacetate
13.69	isooctaan
13.71	1,2-Dichloroethane
13.72	Cyclohexene
13.81	Tert-amyl methyl ether (TAME)
14.09	n-Heptane
14.19	3-Methyl-2-butanone
14.71	1-Butanol
14.75	Propylene glycol monomethyl ether (PGME)
14.80	1,1-Dichloropropane
14.93	Trichloroethylene
15.14	Ethyl acrylate
15.34	Methyl propyl ketone
15.42	Methylcyclohexane
15.54	1,2-Dichloropropane
15.58	2,3-dichloropropene

(Table 11 continuing)

RT (min)	Compound
15.58	Ethylpropionate
15.62	Methyl methacrylate
15.64	3-Pentanone
15.68	1,4-Dioxane
15.74	Dibromomethane
15.76	n-Propyl acetate
15.85	Ethylene chlorohydrine
15.91	2-Pentanol
15.93	3-Pentanol
16.11	Dichlorobromomethane
16.38	2-Ethoxyethanol
16.86	Epichlorohydrine
17.08	cis-1,3-Dichloropropene
17.39	Methyl isobutyl keton
17.49	3-Methyl-1-butanol
17.80	Toluene
18.04	n-Octane
18.06	Isobutyl acetate
18.22	Methyl isobutyl carbinol
18.31	Isopropyl glycol
18.36	trans-1,3-Dichloropropene
18.43	Ethyl methacrylate
18.61	Ethylene glycol diethyl ether
18.63	Pentanol
18.82	1,1,2-Trichloroethane
18.94	Tetrachloroethylene
19.18	2,4-Dimethyl-3-pentanone
19.20	1,3-Dichloropropane
19.28	Methyl-n-butyl ketone
19.52	n-Butyl acetate
19.53	Mesityl oxide
19.63	Tetrahydrothiophene
19.68	Dibromochloromethane
19.84	Cyclopentanone
19.91	2-Propoxyethanol
19.96	4-Vinyl-1-cyclohexene
19.97	1,2-Dibromoethane
20.28	Dimethyl formamide
20.68	Ethylene glycol methylether acetate
21.07	Chlorobenzene
21.14	Isopropyl glycidyl ether
21.26	Dibutyl ether
21.29	Ethyl benzene
21.33	1,1,1,2-Tetrachloroethane
21.57	1-Methoxy-2-propanol acetate (PGMEA)
21.60	m-Xylene + p-Xylene
21.61	Furfural
21.62	n-Nonane
21.72	Methyl isoamyl ketone
21.72	Isopentylacetate
22.05	4-Heptanone
22.11	4-Hydroxy-4-methyl-2-pentanone
22.26	1-Broom-3-chloropropane
22.40	Butyl acrylate
22.43	Furfuryl alcohol
22.51	o-Xylene
22.56	3-Heptanone
22.57	Styrene
22.67	Butylpropionate
22.78	Methyl amyl ketone
22.84	2-Ethoxyethyl acetate
22.92	n-Amyl acetate
23.04	Tribromomethane (Bromoform)
23.04	Cyclohexanol
23.23	N,N-Dimethylacetamide
23.36	α-Pinene
23.37	Ethylene glycol monobutylether
23.39	3-Ethyltoluene
23.39	Cumene
23.86	Cyclohexanone

(Table 11 continuing)

RT (min)	Compound
24.15	1,1,2,2-Tetrachloroethane
24.19	Bromobenzene
24.33	1,2,3-Trichloropropane
24.35	5-Methyl-3-heptanone
24.40	Propylbenzene
24.66	2-Chlorotoluene
24.71	4-Ethyltoluene
24.73	trans-2-Methylcyclohexanol
24.85	1,3,5-Trimethylbenzene
24.85	n-Decane
24.92	cis-2-Methylcyclohexanol
24.95	4-Chlorotoluene
25.01	Bultylmethacrylate
25.02	cis-4-Methylcyclohexanol
25.10	trans-4-methylcyclohexanol
25.18	Di-iso-butyl ketone
25.27	2-Methylcyclohexanone
25.30	2-Ethyltoluene
25.39	α-Methylstyrene
25.57	3-Methylcyclohexanone
25.62	Tert-butylbenzene
25.71	Pentachloroethane
25.74	Butyl glycidyl ether
25.78	1,2,4-Trimethylbenzene
25.79	4-Methylcyclohexanone
26.05	Ethylene glycoldiacetate
26.11	Isobutyl benzene
26.16	sec-Butylbenzene
26.25	Dichloroethyl ether
26.43	D-Limonene
26.48	1,3-Dichlorobenzene
26.56	1-Methyl-4-isopropylbenzene
26.74	1,4-Dichlorobenzene
26.78	Dipropyleenglycol methyl ether
26.79	1,2,3-Trimethylbenzene
27.04	Benzyl chloride
27.25	1,3-Diethylbenzene
27.51	1,4-Diethylbenzene
27.56	Butylbenzene
27.60	trans-Decaline
27.62	1,2-Dichlorobenzene
27.74	1,2-Diethylbenzene
27.82	Undecane
27.91	Diethylene glycol diethyl ether
28.29	Hexachloroethane
28.40	2-Butoxy ethyl acetate
28.41	Benzyl alcohol
28.57	Tert-Butyltoluene
29.02	1-Methyl-2-pyrrolidone
29.02	cis-Decaline
29.62	1,2-Dibromo-3-chloropropane
30.02	1,3,5-Trichlorobenzene
30.59	Dodecane
30.67	1,4-Diisolpropylbenzene
31.10	1,2,3,4-Tetrahydronaftalene
31.13	Isoforon
31.16	Benzyl acetate
31.62	1,2,4-Trichlorobenzene
31.95	Hexachlorobutadiene
32.31	Naphthalene
32.84	1,2,3-Trichlorobenzene
33.13	Tridecane
33.57	1,3-Diisopropenylbenzene
35.56	Tetradecane
37.82	Pentadecane
39.94	Hexadecane

Table 12. Recovery efficiency expressed in percentages, measured on 3 concentration levels, the average recoveries and standard deviations were calculated for each compound. Data collected was measured on GC-MS system 1, n=3.

Compound	0.1 mg/L						2.0 mg/L						10.0 mg/L					
	c(Spiked) mg/L	M_1	M_2	M_3	AVG	SD	c(Spiked) mg/L	M_1	M_2	M_3	AVG	SD	c(Spiked) mg/L	M_1	M_2	M_3	AVG	SD
1,1,1,2-Tetrachloorethaan	0.10	294.3	98.7	85.8	**159.6**	**116.82**	2.00	101.4	98.2	98.0	**99.2**	**1.90**	10.00	96.9	85.9	118.8	**100.5**	**16.73**
1,1,1-Trichloorethaan	0.10	560.2	93.8	84.6	**246.2**	**271.95**	2.00	101.3	97.6	95.9	**98.3**	**2.75**	10.00	90.2	77.4	116.2	**94.6**	**19.73**
1,1,2,2-Tetrachloorethaan	0.10	118.5	71.6	62.7	**84.3**	**29.98**	2.00	63.8	64.5	61.2	**63.2**	**1.75**	10.00	67.5	62.4	85.1	**71.7**	**11.92**
1,1,2-Trichloor-1,2,2-trifluorethaan	0.10	687.1	86.3	105.1	**292.8**	**341.56**	2.00	102.1	82.3	98.9	**94.4**	**10.67**	10.00	75.1	47.0	85.2	**69.1**	**19.76**
1,1,2-Trichloorethaan	0.10	271.0	94.7	75.1	**146.9**	**107.90**	2.00	97.0	97.1	88.9	**94.4**	**4.71**	10.00	79.7	73.9	109.4	**87.7**	**19.01**
1,1-Dichloorethaan	0.10	619.3	89.5	85.5	**264.7**	**307.04**	2.00	93.3	90.7	95.9	**93.3**	**2.64**	10.00	80.2	63.9	99.0	**81.0**	**17.55**
1,1-Dichlooretheen	0.10	664.9	93.9	93.5	**284.1**	**329.83**	2.00	96.7	86.3	95.4	**92.8**	**5.64**	10.00	90.3	65.4	103.3	**86.3**	**19.26**
1,1-Dichloorpropaan	0.10	485.1	101.4	87.3	**224.6**	**225.71**	2.00	98.6	97.8	94.0	**96.8**	**2.43**	10.00	86.9	78.1	114.9	**93.3**	**19.22**
1,1-Dichloorpropeen	0.10	549.0	96.2	84.5	**243.2**	**264.86**	2.00	98.4	97.6	93.5	**96.5**	**2.64**	10.00	93.2	82.2	122.4	**99.3**	**20.74**
1,2,3,4-Tetrahydronaftaleen	0.12	126.8	77.0	57.9	**87.2**	**35.60**	2.43	91.4	101.3	81.4	**91.4**	**9.97**	12.13	77.4	75.8	103.9	**85.7**	**15.80**
1,2,3-Trichloorbenzeen	0.10	90.4	56.2	43.7	**63.4**	**24.18**	2.00	60.4	68.9	56.4	**61.9**	**6.40**	10.00	51.2	48.6	75.3	**58.4**	**14.72**
1,2,3-Trichloorpropaan	0.10	153.6	83.9	66.1	**101.2**	**46.27**	2.00	89.7	95.4	84.1	**89.7**	**5.66**	10.00	79.4	76.1	118.3	**91.3**	**23.49**
1,2,3-Trimethylbenzeen	0.10	201.2	82.0	67.0	**116.7**	**73.54**	2.00	89.7	94.0	89.7	**91.2**	**2.50**	10.00	87.8	82.0	123.0	**97.6**	**22.23**
1,2,4-Trichloorbenzeen	0.10	113.8	66.6	51.2	**77.2**	**32.64**	2.00	71.5	80.3	66.2	**72.7**	**7.11**	10.00	58.2	55.4	88.2	**67.3**	**18.16**
1,2,4-Trimethylbenzeen	0.10	226.3	82.2	71.6	**126.7**	**86.40**	2.00	95.0	98.1	94.0	**95.7**	**2.11**	10.00	92.6	84.8	127.9	**101.8**	**22.97**
1,2-Dibroom-3-chloorpropaan	0.10	101.6	60.9	49.8	**70.8**	**27.24**	2.00	70.3	72.0	64.4	**68.9**	**4.02**	10.00	82.3	75.6	103.9	**87.3**	**14.81**
1,2-Dibroomethaan	0.10	349.7	93.3	80.7	**174.6**	**151.83**	2.00	98.6	96.4	96.1	**97.0**	**1.35**	10.00	91.8	81.3	114.4	**95.8**	**16.91**
1,2-Dichloorbenzeen	0.10	150.2	77.9	59.0	**95.7**	**48.13**	2.00	82.1	89.6	76.4	**82.7**	**6.61**	10.00	70.4	68.1	108.6	**82.4**	**22.73**
1,2-Dichloorethaan	0.10	509.3	119.2	109.3	**245.9**	**228.16**	2.00	94.9	96.0	91.8	**94.2**	**2.20**	10.00	76.6	70.1	99.7	**82.2**	**15.57**
1,2-Dichloorpropaan	0.10	455.6	95.4	80.9	**210.6**	**212.28**	2.00	101.5	99.8	93.5	**98.3**	**4.22**	10.00	88.1	78.2	114.3	**93.5**	**18.67**
1,2-Diethylbenzeen	0.10	163.6	84.8	65.6	**104.7**	**51.94**	2.00	100.2	110.5	91.8	**100.8**	**9.37**	10.00	86.1	83.5	114.0	**94.5**	**16.92**
1,3,5-Trichloorbenzeen	0.10	153.9	80.4	62.1	**98.8**	**48.64**	2.00	84.0	92.5	77.8	**84.8**	**7.39**	10.00	69.1	65.6	106.3	**80.3**	**22.54**
1,3,5-Trimethylbenzeen	0.10	263.9	91.4	74.9	**143.4**	**104.67**	2.00	98.2	102.0	97.7	**99.3**	**2.38**	10.00	95.3	88.6	131.0	**105.0**	**22.80**
1,3-Butadiene	0.10	-	-	-	-	-	2.00	84.9	83.4	78.3	**82.2**	**3.51**	10.00	77.3	52.5	95.6	**75.1**	**21.64**
1,3-Dichloorbenzeen	0.10	187.2	85.4	66.9	**113.2**	**64.77**	2.00	89.3	96.8	83.0	**89.7**	**6.92**	10.00	76.3	72.7	117.5	**88.9**	**24.87**
1,3-Dichloorpropaan	0.10	340.5	91.4	101.5	**177.8**	**141.02**	2.00	99.8	100.9	100.8	**100.5**	**0.61**	10.00	83.2	77.3	118.0	**92.9**	**22.01**
1,3-Diethylbenzeen	0.10	163.6	86.2	66.7	**105.5**	**51.25**	2.00	104.5	116.3	94.6	**105.1**	**10.82**	10.00	87.6	87.0	117.1	**97.2**	**17.23**
1,3-Diisopropylbenzeen	0.12	43.4	34.5	16.4	**31.4**	**13.76**	2.31	66.0	79.2	50.2	**65.1**	**14.52**	11.57	59.3	61.6	91.0	**70.6**	**17.67**
1,4-Dichloorbenzeen	0.10	175.3	84.0	66.0	**108.4**	**58.62**	2.00	86.9	94.7	80.1	**87.2**	**7.32**	10.00	74.6	70.7	114.3	**86.5**	**24.15**
1,4-Diethylbenzeen	0.10	167.2	84.4	61.9	**104.5**	**55.44**	2.00	105.2	115.3	94.5	**105.0**	**10.39**	10.00	88.1	86.1	141.0	**105.1**	**31.10**
1,4-Diisopropylbenzeen	0.11	117.0	83.0	64.6	**88.2**	**26.56**	2.14	102.5	113.2	91.7	**102.4**	**10.75**	10.72	85.2	83.4	138.2	**102.3**	**31.11**
1,4-Dioxane	0.13	202.9	75.2	64.0	**114.0**	**77.18**	2.59	85.8	81.8	79.8	**82.5**	**3.08**	12.93	82.1	73.2	103.8	**86.4**	**15.75**
1-Broom-3-chloorpropaan	0.20	219.0	81.8	79.2	**126.7**	**79.97**	3.98	98.6	103.5	89.6	**97.2**	**7.02**	19.90	80.6	77.5	116.4	**91.5**	**21.65**
1-Methyl-2-pyrrolidon	0.13	-	-	-	-	-	2.58	-	-	-	-	-	12.88	-	-	-	-	-
1-Pentanol	0.10	-	-	-	-	-	2.04	44.1	39.2	31.3	**38.2**	**6.46**	10.18	57.6	51.7	61.5	**56.9**	**4.93**
2,2-Dichloorpropaan	0.10	714.0	102.5	93.6	**303.4**	**355.64**	2.00	97.7	92.8	100.2	**96.9**	**3.76**	10.00	101.4	81.2	109.0	**97.2**	**14.40**
2,2-Dimethylbutaan	0.10	709.6	97.8	114.7	**307.4**	**348.45**	1.98	102.2	90.4	99.7	**97.4**	**6.23**	9.89	84.8	60.2	112.9	**86.0**	**26.39**
2,3-Dichloorpropeen	0.10	482.6	88.3	83.5	**218.1**	**229.03**	2.00	95.0	90.7	97.4	**94.3**	**3.42**	10.00	96.4	84.4	112.2	**97.7**	**13.91**
2,4-Dimethyl-3-pentanon	0.10	206.6	89.9	74.1	**123.6**	**72.36**	2.02	102.9	105.1	93.3	**100.4**	**6.29**	10.08	93.2	87.9	129.1	**103.4**	**22.41**
2,4-Dimethylpentaan	0.09	550.7	100.6	81.6	**244.3**	**265.52**	1.74	101.4	100.8	93.5	**98.6**	**4.43**	8.72	100.1	85.2	132.1	**105.8**	**23.96**
2-Butanol	0.10	94.4	55.1	40.3	**63.3**	**27.99**	2.02	48.9	45.7	45.4	**46.7**	**1.93**	10.08	56.9	46.4	50.1	**51.2**	**5.35**
2-Butoxy ethyl acetaat	0.12	-	-	-	-	-	2.35	30.7	33.1	21.5	**28.4**	**6.13**	11.75	92.9	88.8	109.4	**97.0**	**10.94**
2-Chloor-1,3-butadiene	0.10	328.6	14.6	0.0	**114.4**	**185.65**	2.00	80.6	80.5	77.1	**79.4**	**2.01**	10.00	94.3	80.9	121.8	**99.0**	**20.87**
2-Chloortolueen	0.10	259.5	85.7	76.2	**140.5**	**103.18**	2.00	90.5	93.4	90.1	**91.3**	**1.81**	10.00	88.9	80.7	119.0	**96.2**	**20.19**
2-Ethoxyethanol	0.12	-	-	-	-	-	2.33	24.9	24.0	18.3	**22.4**	**3.58**	11.63	43.8	49.3	58.6	**50.6**	**7.48**
2-Ethoxyethyl acetaat	0.12	-	-	-	-	-	2.43	44.2	42.7	30.0	**39.0**	**7.79**	12.17	98.6	89.3	130.4	**106.1**	**21.55**
2-Ethyltolueen	0.10	241.7	87.3	73.8	**134.2**	**93.31**	2.00	95.6	98.7	95.0	**96.4**	**1.97**	10.00	94.1	86.2	129.3	**103.2**	**22.94**
2-Methoxyethanol (methyl cellosolve)	0.12	162.4	55.2	40.8	**86.1**	**66.45**	2.41	86.3	83.5	74.4	**81.4**	**6.22**	12.07	83.3	75.8	96.8	**85.3**	**10.64**
2-Methyl-1-propanol	0.10	82.5	41.1	46.7	**56.8**	**22.47**	2.01	42.4	41.2	37.2	**40.3**	**2.69**	10.03	48.8	40.9	46.4	**45.4**	**4.04**
2-Methyl-2-butanol	0.10	234.3	151.0	144.9	**176.8**	**49.95**	2.04	57.1	55.3	55.3	**55.9**	**1.04**	10.19	70.1	62.9	79.4	**70.8**	**8.28**
2-Methylbutaan	0.08	753.0	437.5	461.5	**550.7**	**175.65**	1.54	87.2	111.6	94.4	**97.7**	**12.55**	7.70	52.2	41.9	81.8	**58.6**	**20.70**
2-Methylcyclohexanon	0.12	48.4	46.6	39.8	**45.0**	**4.54**	2.31	63.8	67.8	55.1	**62.2**	**6.49**	11.55	91.5	88.5	144.6	**108.2**	**31.54**
2-Methylpentaan	0.08	1181.4	121.4	141.6	**481.5**	**606.23**	1.63	86.1	96.2	108.7	**97.0**	**11.32**	8.17	113.7	67.8	82.7	**88.1**	**23.44**
2-Pentanol	0.10	53.4	50.0	45.1	**49.5**	**4.17**	2.03	48.5	46.8	41.4	**45.6**	**3.68**	10.15	61.6	57.4	63.0	**60.7**	**2.88**
2-Propoxyethanol	0.11	-	-	-	-	-	2.28	25.5	24.7	15.5	**21.9**	**5.55**	11.39	60.0	62.8	69.9	**64.2**	**5.08**
3-Chloor-1-propeen (allylchloride)	0.10	-	-	-	-	-	2.00	-	-	-	-	-	10.00	-	-	-	-	-
3-Ethyltolueen	0.10	312.3	97.2	81.0	**163.5**	**129.13**	2.00	100.2	102.1	98.8	**100.4**	**1.67**	10.00	97.6	90.0	131.4	**106.3**	**22.04**
3-Heptanon	0.10	107.9	81.5	58.3	**82.6**	**24.80**	2.03	100.0	104.5	87.5	**97.3**	**8.81**	10.15	92.2	89.3	126.9	**102.8**	**20.87**
3-methyl-1-Butanol	0.10	37.5	33.6	19.9	**30.3**	**9.23**	2.03	36.4	35.7	29.0	**33.7**	**4.05**	10.13	54.7	49.6	62.5	**55.6**	**6.52**
3-Methyl-2-butanon	0.10	319.8	92.2	80.0	**164.0**	**135.05**	2.01	96.7	96.3	94.7	**95.9**	**1.08**	10.07	95.6	85.7	123.6	**101.6**	**19.68**
3-Methylcyclohexanon	0.11	-	-	-	-	-	2.29	49.6	52.5	40.8	**47.7**	**6.06**	11.43	84.8	82.1	130.3	**99.1**	**27.08**
3-Pentanol	0.10	62.8	49.1	34.1	**48.7**	**14.34**	2.04	54.4	51.3	46.4	**50.7**	**4.01**	10.19	65.0	58.9	74.8	**66.2**	**7.98**
3-Pentanon	0.10	260.3	85.0	65.3	**136.9**	**107.38**	2.04	98.8	100.6	92.3	**97.2**	**4.38**	10.19	89.6	84.0	108.1	**93.9**	**12.61**
4-Chloortolueen	0.10	234.2	82.9	71.9	**129.7**	**90.70**	2.00	90.6	93.1	91.2	**91.6**	**1.32**	10.00	89.2	80.7	121.0	**96.9**	**21.25**
4-Ethyltolueen	0.10	267.7	91.2	74.3	**144.4**	**107.12**	2.00	100.0	103.0	99.8	**100.9**	**1.76**	10.00	97.1	89.3	133.3	**106.6**	**23.51**
4-Heptanon	0.10	117.1	72.6	54.9	**81.5**	**32.05**	2.05	99.3	102.9	87.7	**96.6**	**7.91**	10.25	91.4	89.3	118.4	**99.7**	**16.24**
4-Hydroxy-4-methyl-2-pentanon	0.12	-	-	-	-	-	2.33	-	-	-	-	-	11.64	-	-	-	-	-
4-Methylcyclohexanon	0.11	-	-	-	-	-	2.29	48.3	51.8	37.9	**46.0**	**7.20**	11.43	83.4	82.0	127.7	**97.7**	**26.02**
4-Vinyl-1-cyclohexeen	0.10	370.8	96.6	76.2	**181.2**	**164.49**	2.08	106.1	111.2	93.9	**103.7**	**8.91**	10.38	92.5	88.7	112.5	**97.9**	**12.78**
5-methyl-3-heptanon	0.10	100.7	76.6	51.9	**76.4**	**24.38**	2.06	93.5	100.3	81.4	**91.7**	**9.58**	10.29	90.1	88.8	140.7	**106.5**	**29.60**
Aceton	0.10	800.2	254.2	422.1	**492.2**	**279.70**	1.96	81.1	68.1	92.6	**80.6**	**12.23**	9.80	97.8	64.1	67.5	**76.5**	**18.54**
Allyl alcohol	0.11	-	-	-	-	-	2.14	32.6	26.6	29.3	**29.5**	**2.98**	10.68	30.6	20.5	22.9	**24.7**	**5.28**
a-Methylstyreen	0.11	122.5	50.8	30.3	**67.9**	**48.45**	2.28	93.9	101.9	79.0	**91.6**	**11.63**	11.38	83.2	81.7	106.4	**90.4**	**13.85**
a-Pineen	0.11	324.4	107.5	80.3	**170.7**	**133.77**	2.15	104.9	112.9	93.6	**103.8**	**9.67**	10.73	85.9	82.7	133.1	**100.5**	**28.22**
Benzeen	0.10	815.9	664.4	652.1	**710.8**	**91.24**	2.00	67.6	67.3	65.9	**66.9**	**0.90**	10.00	65.0	63.1	77.4	**68.5**	**7.77**
Benzyl acetaat	0.13	20.1	23.3	21.4	**21.6**	**1.61**	2.63	32.0	33.8	22.3	**29.3**	**6.18**	13.13	74.8	69.6	101.0	**81.8**	**16.85**
Benzyl alcohol	0.13	-	-	-	-	-	2.60	-	-	-	-	-	13.00	24.4	27.2	26.2	**25.9**	**1.38**
Benzyl chloride	0.14	113.8	71.5	53.6	**79.6**	**30.94**	2.75	96.2	99.8	78.5	**91.5**	**11.40**	13.75	86.7	82.4	124.2	**97.8**	**22.98**
Broombenzeen	0.10	257.5	87.0	74.4	**139.6**	**102.28**	2.00	89.8	91.9	89.7	**90.5**	**1.26**	10.00	88.3	81.0	119.0	**96.1**	**20.20**
Broomchloormethaan	0.10	536.0	89.5	82.7	**236.1**	**259.78**	2.00	91.3	91.1	89.4	**90.6**	**1.03**	10.00	69.1	58.5	84.0	**70.6**	**12.80**
Broomdichloormethaan	0.10	437.9	90.7	86.6	**205.1**	**201.63**	2.00	92.6	90.0	95.6	**92.7**	**2.82**	10.00	82.7	73.9	97.3	**84.6**	**11.84**
Broommethaan	0.10	195.0	95.0	85.3	**125.1**	**60.74**	2.00	52.2	56.3	29.0	**45.8**	**14.71**	10.00	31.0	20.4	29.8	**27.1**	**5.80**
Butyl glycidil ether	0.11	-	-	-	-	-	2.28	59.1	62.7	46.7	**56.1**	**8.41**	11.38	89.4	92.5	117.3	**99.8**	**15.29**
Butylacrylaat	0.11	116.5	69.3	54.2	**80.0**	**32.52**	2.24	104.7	108.3	87.2	**100.1**	**11.28**	11.18	92.9	89.6	108.5	**97.0**	**10.07**
Butylbenzeen	0.10	214.4	91.9	78.1	**128.1**	**75.04**	2.00	99.8	105.2	99.6	**101.5**	**3.15**	10.00	95.3	89.0	133.8	**106.0**	**24.28**
Butylmethacrylaat	0.11	84.2	63.9	43.4	**63.8**	**20.40**	2.24	105.1	109.7	85.6	**100.2**	**12.79**	11.18	97.9	93.1	147.6	**112.8**	**30.19**
Butylpropionaat	0.11	118.9	74.2	53.7	**82.2**	**33.32**	2.19	107.2	107.0	90.8	**101.7**	**9.40**	10.94	97.2	88.8	135.9	**107.3**	**25.13**
Chloorethaan	0.10	614.3	139.6	139.6	**297.8**	**274.07**	2.00	88.8	91.9	71.8	**84.2**	**10.83**	10.00	45.2	28.0	44.2	**39.1**	**9.65**
Chloormethaan	0.10	635.0	171.0	345.9	**384.0**	**234.34**	2.00	65.1	51.0	14.0	**43.4**	**26.39**	10.00	29.3	15.1	45.8	**30.1**	**15.33**

(Table 12 continuing)

Compound	0.1 mg/L						2.0 mg/L						10.0 mg/L					
	c(Spiked) mg/L	M_1	M_2	M_3	AVG	SD	c(Spiked) mg/L	M_1	M_2	M_3	AVG	SD	c(Spiked) mg/L	M_1	M_2	M_3	AVG	SD
cis-1,3-Dichloorpropeen	0.10	368.6	96.1	79.0	**181.2**	**162.49**	2.00	100.1	100.4	90.8	**97.1**	**5.46**	10.00	83.9	77.7	109.4	**90.4**	**16.78**
cis-2-Methylcyclohexanol	0.12	-	-	-	-	-	2.34	30.7	31.7	20.9	**27.8**	**5.95**	11.70	65.6	63.8	80.9	**70.1**	**9.38**
cis-4-Methylcyclohexanol	0.11	-	-	-	-	-	2.29	31.7	32.9	21.9	**28.8**	**6.02**	11.47	55.4	55.7	72.9	**61.3**	**10.05**
cis-Decalin	0.11	229.4	94.9	70.7	**131.7**	**85.47**	2.24	102.7	115.2	94.3	**104.1**	**10.54**	11.20	85.7	83.8	139.0	**102.8**	**31.33**
Cumeen	0.10	261.8	98.3	75.3	**145.2**	**101.68**	2.00	103.5	110.9	93.6	**102.7**	**8.69**	10.00	88.6	85.9	135.5	**103.3**	**27.90**
Cyclohexaan	0.10	615.8	142.9	211.6	**323.4**	**255.51**	1.95	101.4	101.0	97.8	**100.1**	**1.98**	9.74	84.8	73.1	113.9	**90.6**	**20.98**
Cyclohexanol	0.12	-	-	-	-	-	2.41	17.6	19.7	13.0	**16.7**	**3.39**	12.03	52.5	49.7	61.0	**54.4**	**5.88**
Cyclohexanon	0.12	-	-	-	-	-	2.37	51.9	54.4	44.1	**50.1**	**5.36**	11.85	79.0	77.8	121.5	**92.8**	**24.85**
Cyclohexeen	0.10	796.0	410.0	423.2	**543.0**	**219.14**	2.03	84.0	88.2	74.4	**82.2**	**7.07**	10.14	78.1	92.2	76.2	**82.2**	**8.74**
Cyclopentaan	0.09	792.3	139.0	143.4	**358.2**	**375.91**	1.88	76.6	88.2	99.4	**88.1**	**11.40**	9.40	84.1	45.3	87.6	**72.3**	**23.47**
Cyclopentanon	0.12	68.9	43.4	52.8	**55.0**	**12.89**	2.38	68.5	66.7	61.1	**65.4**	**3.85**	11.88	76.8	70.2	170.6	**105.9**	**56.14**
Dibroomchloormethaan	0.10	291.1	95.4	79.5	**155.3**	**117.85**	2.00	96.7	93.9	92.4	**94.3**	**2.20**	10.00	85.4	78.2	102.7	**88.8**	**12.63**
Dibroommethaan	0.10	479.9	90.9	83.4	**218.1**	**226.81**	2.00	90.4	87.6	93.4	**90.5**	**2.90**	10.00	76.8	67.8	89.9	**78.2**	**11.11**
Dibutyl ether	0.10	220.2	88.5	67.2	**125.3**	**82.84**	1.93	106.8	112.2	95.2	**104.7**	**8.71**	9.63	94.5	90.9	118.5	**101.3**	**15.00**
Dichloordifluormethaan	0.10	463.6	154.8	170.8	**263.1**	**173.87**	2.00	62.6	58.9	31.0	**50.8**	**17.26**	10.00	8.1	5.2	19.4	**10.9**	**7.51**
Dichloorethyl ether	0.15	67.6	54.9	42.5	**55.0**	**12.53**	3.05	66.2	70.6	58.2	**65.0**	**6.25**	15.25	77.1	75.0	102.5	**84.9**	**15.33**
Dichloormethaan	0.10	726.3	90.9	132.0	**316.4**	**355.56**	2.00	84.1	81.0	93.5	**86.2**	**6.53**	10.00	73.7	44.8	70.6	**63.0**	**15.87**
Diethyleen glycol diethyl ether	0.11	0.0	0.0	0.0	**0.0**	**0.00**	2.27	11.5	13.8	8.0	**11.1**	**2.96**	11.37	85.0	80.4	121.8	**95.7**	**22.65**
Diisobutyl keton	0.10	86.3	62.8	47.2	**65.4**	**19.70**	2.01	95.8	104.9	84.9	**95.2**	**10.05**	10.03	90.0	91.9	118.9	**100.3**	**16.16**
Diisopropylether	0.10	549.3	86.1	86.4	**240.6**	**267.36**	2.00	96.9	95.0	97.9	**96.6**	**1.46**	10.00	103.7	84.4	130.2	**106.1**	**22.97**
Dimethyl formamide	0.12	-	-	-	-	-	2.36	-	-	-	-	-	11.80	-	-	-	-	-
Dipropyleenglycol methyl ether	0.12	-	-	-	-	-	2.30	-	-	-	-	-	11.50	0.0	0.0	0.0	**0.0**	**0.00**
D-Limoneen	0.11	194.5	86.3	64.6	**115.2**	**69.59**	2.10	114.1	122.5	96.6	**111.1**	**13.23**	10.50	92.5	91.9	150.8	**111.7**	**33.85**
Dodecaan	0.09	215.3	128.3	100.1	**147.9**	**60.03**	1.88	121.3	134.3	102.7	**119.4**	**15.89**	9.38	92.1	89.2	121.0	**100.8**	**17.61**
EPI (Epichloorhydrine)	0.15	226.7	79.6	67.7	**124.7**	**88.59**	2.95	89.6	88.8	83.6	**87.4**	**3.27**	14.77	69.7	62.7	88.5	**73.6**	**13.31**
ETBE	0.10	515.2	88.3	84.1	**229.2**	**247.72**	2.00	99.5	97.4	99.3	**98.7**	**1.13**	10.00	100.1	85.1	130.9	**105.4**	**23.32**
Ethanol	0.10	243.2	127.5	188.4	**186.4**	**57.88**	1.97	33.9	24.1	31.1	**29.7**	**5.04**	9.87	29.6	20.7	17.3	**22.5**	**6.34**
Ethyl acetaat	0.11	510.6	118.4	187.6	**272.2**	**209.34**	2.26	97.0	96.0	104.0	**99.0**	**4.39**	11.28	92.9	76.9	84.6	**84.8**	**8.02**
Ethyl propionaat	0.11	324.0	66.7	66.3	**152.3**	**148.65**	2.21	105.5	101.0	94.0	**100.2**	**5.82**	11.05	93.7	82.5	120.9	**99.0**	**19.75**
Ethylacrylaat	0.12	313.0	77.9	66.5	**152.5**	**139.17**	2.35	99.2	97.4	92.9	**96.5**	**3.26**	11.75	93.7	85.4	100.3	**93.1**	**7.45**
Ethylbenzeen	0.10	314.1	102.6	80.6	**165.8**	**128.92**	2.00	102.3	108.4	93.2	**101.3**	**7.68**	10.00	89.0	86.1	131.6	**102.2**	**25.47**
Ethyleen chloorhydrin	0.15	-	-	-	-	-	3.00	14.7	14.8	36.0	**21.9**	**12.26**	15.00	19.9	9.5	48.0	**25.8**	**19.94**
Ethyleen glycol diethyl ether	0.11	76.9	49.0	43.3	**56.4**	**17.98**	2.10	91.1	92.1	79.9	**87.7**	**6.80**	10.50	92.3	89.4	130.9	**104.2**	**23.19**
Ethyleen glycol dimethyl ether	0.11	167.5	53.8	41.6	**87.6**	**69.46**	2.17	86.4	81.1	74.6	**80.7**	**5.87**	10.85	83.4	73.6	82.0	**79.6**	**5.28**
Ethyleen glycol methylether acetaat	0.13	-	-	-	-	-	2.53	59.1	54.5	42.9	**52.2**	**8.33**	12.63	97.4	87.2	104.5	**96.4**	**8.70**
Ethyleen glycol monobutyl ether	0.11	-	-	-	-	-	2.25	0.0	0.0	0.0	**0.0**	**0.00**	11.25	0.0	0.0	116.4	**38.8**	**67.21**
Ethyleen glycoldiacetaat	0.14	-	-	-	-	-	2.75	21.4	18.5	11.3	**17.1**	**5.16**	13.75	86.3	86.4	91.8	**88.1**	**3.13**
Ethylether	0.10	681.3	102.5	108.9	**297.6**	**332.36**	2.00	103.9	85.8	98.5	**96.1**	**9.32**	10.00	96.6	67.7	110.2	**91.5**	**21.69**
Ethylmethacrylaat	0.10	267.2	79.9	68.4	**138.5**	**111.64**	2.00	103.0	97.8	96.5	**99.1**	**3.48**	10.00	104.8	92.4	125.0	**107.4**	**16.45**
Furfural	0.15	-	-	-	-	-	2.90	41.9	41.8	33.5	**39.1**	**4.79**	14.50	52.0	51.0	78.6	**60.5**	**15.64**
Furfuryl alcohol	0.14	-	-	-	-	-	2.83	45.5	43.5	20.9	**36.6**	**13.62**	14.13	42.4	40.4	36.6	**39.8**	**2.91**
Hexachloorbutadieen	0.10	164.2	93.4	79.1	**112.2**	**45.54**	2.00	85.7	93.1	88.4	**89.1**	**3.71**	10.00	83.7	78.1	117.6	**93.1**	**21.38**
Hexachloorethaan	0.10	212.5	91.8	88.6	**131.0**	**70.61**	2.00	89.9	94.1	94.5	**92.8**	**2.57**	10.00	85.7	77.8	122.6	**95.4**	**23.94**
Hexadecaan	0.10	66.9	79.3	58.7	**68.3**	**10.36**	1.93	98.9	118.8	89.9	**102.5**	**14.79**	9.67	71.2	69.5	91.8	**77.5**	**12.39**
Iodomethaan	0.10	212.0	53.7	45.3	**103.7**	**93.92**	2.00	61.6	59.6	50.0	**57.0**	**6.20**	10.00	54.3	39.1	45.2	**46.2**	**7.66**
Isobutyl acetaat	0.11	231.7	72.9	74.0	**126.2**	**91.35**	2.19	108.5	105.2	91.8	**101.8**	**8.83**	10.94	95.7	87.0	108.0	**96.9**	**10.57**
Isobutyl benzeen	0.11	194.4	90.4	66.5	**117.1**	**67.99**	2.13	103.3	111.8	93.2	**102.8**	**9.33**	10.67	88.8	85.7	138.5	**104.3**	**29.65**
Isoforon	0.12	-	-	-	-	-	2.30	12.3	14.9	9.4	**12.2**	**2.74**	11.50	61.9	62.6	90.3	**71.6**	**16.21**
Isooctaan	0.09	-	-	-	-	-	1.73	-	-	-	-	-	8.63	-	-	-	-	-
Isopentyl acetaat	0.11	121.3	68.4	52.5	**80.7**	**36.01**	2.19	105.7	104.0	90.0	**99.9**	**8.66**	10.95	97.1	87.8	135.4	**106.8**	**25.23**
Isopropyl acetaat	0.11	357.9	93.5	76.3	**175.9**	**157.86**	2.18	104.2	103.0	98.2	**101.8**	**3.17**	10.88	93.9	83.6	98.7	**92.1**	**7.70**
Isopropyl glycidil ether	0.12	71.3	56.3	40.7	**56.1**	**15.28**	2.31	70.0	70.3	57.1	**65.8**	**7.51**	11.55	91.8	86.8	127.0	**101.9**	**21.94**
Isopropyl glycol	0.11	-	-	-	-	-	2.26	18.0	17.9	11.1	**15.7**	**3.99**	11.29	63.8	60.0	73.3	**65.7**	**6.88**
MEK (2-Butanone)	0.10	377.0	102.8	101.8	**193.9**	**158.60**	2.01	94.8	90.5	95.0	**93.4**	**2.55**	10.07	99.5	81.1	149.7	**110.1**	**35.50**
Mesityl oxide	0.11	-	-	-	-	-	2.15	-	-	-	-	-	10.73	-	-	-	-	-
Methacrylonitrile	0.10	383.7	76.0	69.4	**176.4**	**179.60**	2.00	90.9	85.0	91.2	**89.0**	**3.50**	10.00	87.7	73.4	110.5	**90.5**	**18.73**
Methyl acrylaat	0.12	439.4	75.1	69.7	**194.7**	**211.93**	2.38	95.4	90.7	95.1	**93.7**	**2.63**	11.88	96.6	81.0	122.1	**99.9**	**20.73**
Methyl amyl keton	0.10	80.4	67.1	49.6	**65.7**	**15.46**	2.00	91.8	97.4	77.7	**89.0**	**10.11**	10.00	98.8	99.3	170.8	**123.0**	**41.43**
Methyl isoamyl keton	0.10	86.1	61.0	56.8	**68.0**	**15.83**	2.01	95.6	97.2	83.1	**91.9**	**7.70**	10.03	98.9	96.3	168.1	**121.1**	**40.69**
Methyl isobutyl carbinol	0.10	47.2	41.2	33.9	**40.8**	**6.66**	2.02	50.2	47.7	40.6	**46.2**	**4.94**	10.10	71.2	63.9	82.3	**72.4**	**9.26**
Methyl isobutyl keton	0.10	196.4	79.8	66.6	**114.3**	**71.46**	2.01	101.1	102.8	90.7	**98.2**	**6.56**	10.03	93.9	88.3	105.4	**95.9**	**8.71**
Methyl propyl keton	0.10	254.1	92.5	81.0	**142.6**	**96.79**	2.02	99.4	98.5	96.2	**98.0**	**1.67**	10.12	96.9	88.5	126.0	**103.8**	**19.65**
Methylal	0.11	-	-	-	-	-	2.15	-	-	-	-	-	10.75	-	-	-	-	-
Methylcyclohexaan	0.10	-	-	-	-	-	1.93	-	-	-	-	-	9.63	-	-	-	-	-
Methylcyclopentaan	0.09	597.6	106.9	96.5	**267.0**	**286.35**	1.87	98.1	98.4	91.3	**95.9**	**4.03**	9.37	88.5	72.7	87.6	**82.9**	**8.86**
Methylmethacrylaat	0.10	388.3	94.3	90.5	**191.0**	**170.82**	2.00	100.7	92.6	99.8	**97.7**	**4.46**	10.00	106.3	92.6	122.9	**107.2**	**15.14**
Methyl-n-butyl keton	0.11	142.2	77.6	67.3	**95.7**	**40.62**	2.20	100.5	101.8	87.4	**96.5**	**7.96**	11.02	95.4	92.0	148.3	**111.9**	**31.59**
Monochloorbenzeen	0.10	297.4	100.1	79.3	**159.0**	**120.38**	2.00	92.7	97.9	87.9	**92.9**	**5.00**	10.00	83.1	78.7	120.7	**94.2**	**23.11**
MTBE	0.10	617.3	81.0	83.3	**260.5**	**308.98**	2.00	94.2	92.6	102.7	**96.5**	**5.45**	10.00	103.7	77.2	127.0	**102.6**	**24.89**
n,n-Dimethylacetamide	0.12	-	-	-	-	-	2.35	-	-	-	-	-	11.75	-	-	-	-	-
Naftaleen	0.10	129.1	69.8	61.7	**86.9**	**36.81**	2.00	69.1	69.0	66.3	**68.1**	**1.56**	10.00	33.1	27.3	39.2	**33.2**	**5.99**
n-Amyl acetaat	0.11	81.8	62.1	50.4	**64.8**	**15.86**	2.19	104.2	105.8	88.8	**99.6**	**9.39**	10.95	98.8	92.9	118.5	**103.4**	**13.43**
n-Butylacetaat	0.11	159.2	72.2	55.7	**95.7**	**55.63**	2.21	104.3	104.6	91.4	**100.1**	**7.56**	11.03	93.7	88.0	127.2	**103.0**	**21.20**
n-Decaan	0.10	348.5	99.5	89.0	**179.0**	**146.89**	2.00	106.1	111.7	106.6	**108.1**	**3.09**	10.00	100.5	95.1	143.1	**112.9**	**26.30**
n-Heptaan	0.10	672.0	129.1	98.5	**299.8**	**322.62**	2.00	101.4	99.2	98.6	**99.7**	**1.51**	10.00	108.1	92.7	127.4	**109.4**	**17.39**
n-Hexaan	0.10	1198.9	291.2	521.9	**670.7**	**471.75**	2.00	99.5	101.8	118.5	**106.6**	**10.34**	10.00	102.0	80.7	136.0	**106.2**	**27.93**
n-Nonaan	0.10	434.1	98.3	87.2	**206.5**	**197.15**	2.00	103.2	102.9	99.5	**101.9**	**2.07**	10.00	104.3	94.5	139.3	**112.7**	**23.55**
n-Octaan	0.10	545.6	103.4	92.3	**247.1**	**258.57**	2.00	101.8	100.2	99.8	**100.6**	**1.04**	10.00	104.1	93.2	133.2	**110.2**	**20.68**
n-Pentaan	0.08	1193.3	882.8	1130.0	**1068.7**	**164.04**	1.57	53.3	46.7	57.0	**52.3**	**5.23**	7.83	59.1	50.7	45.5	**51.8**	**6.87**
n-Propanol	0.10	-	-	-	-	-	2.01	42.4	37.7	35.9	**38.7**	**3.37**	10.04	41.8	32.4	34.1	**36.1**	**5.01**
n-Propyl acetaat	0.11	290.5	90.0	70.4	**150.3**	**121.80**	2.22	102.4	99.7	97.5	**99.8**	**2.45**	11.10	94.9	84.5	100.9	**93.4**	**8.27**
o-Xyleen	0.10	273.5	100.9	78.9	**151.1**	**106.59**	2.00	97.1	102.9	88.8	**96.3**	**7.10**	10.00	84.1	80.8	126.3	**97.1**	**25.35**
p,m-Xyleen	0.10	305.0	101.2	79.8	**162.0**	**124.31**	2.00	100.5	106.3	91.7	**99.5**	**7.37**	10.00	88.0	84.3	130.5	**100.9**	**25.64**
Pentachloorethaan	0.10	58.1	57.0	50.6	**55.2**	**4.06**	2.00	16.1	16.7	12.6	**15.2**	**2.19**	10.00	3.2	2.1	3.9	**3.1**	**0.91**
Pentadecaan	0.10	76.1	81.9	63.3	**73.8**	**9.49**	1.92	113.9	136.8	98.2	**116.3**	**19.40**	9.62	77.7	76.8	97.6	**84.0**	**11.71**
PGME	0.12	-	-	-	-	-	2.30	34.2	32.2	25.6	**30.7**	**4.51**	11.50	55.7	54.5	65.5	**58.6**	**6.00**
PGMEA	0.12	-	-	-	-	-	2.43	60.3	58.7	45.5	**54.9**	**8.12**	12.13	103.4	93.2	109.5	**102.0**	**8.21**
p-isopropyltolueen	0.10	-	-	-	-	-	2.00	-	-	-	-	-	10.00	-	-	-	-	-
Propylbenzeen	0.10	276.0	94.3	80.1	**150.1**	**109.25**	2.00	99.3	102.6	99.5	**100.5**	**1.87**	10.00	96.8	89.5	131.9	**106.1**	**22.69**

(Table 12 continuing)

Compound	0.1 mg/L						2.0 mg/L						10.0 mg/L					
	c(Spiked) mg/L	M_1	M_2	M_3	AVG	SD	c(Spiked) mg/L	M_1	M_2	M_3	AVG	SD	c(Spiked) mg/L	M_1	M_2	M_3	AVG	SD
Styreen	0.10	174.0	60.8	37.6	**90.8**	**73.01**	2.00	86.9	92.1	74.8	**84.6**	**8.88**	10.00	77.3	75.8	114.0	**89.1**	**21.63**
TAME	0.10	524.9	95.5	93.4	**237.9**	**248.50**	2.00	96.7	91.6	99.9	**96.1**	**4.16**	10.00	105.2	90.3	122.0	**105.8**	**15.90**
tert-Butanol	0.10	167.7	50.0	57.1	**91.6**	**65.99**	1.95	52.0	46.4	60.4	**52.9**	**7.04**	9.77	67.3	44.0	47.2	**52.9**	**12.62**
tert-Butylbenzeen	0.10	241.7	94.8	78.1	**138.2**	**89.98**	2.00	98.7	102.0	98.5	**99.7**	**2.00**	10.00	95.5	88.3	132.8	**105.5**	**23.85**
tert-Butyltoluene	0.11	144.5	88.0	67.1	**99.9**	**40.04**	2.15	100.3	110.1	91.2	**100.5**	**9.44**	10.73	85.3	83.3	114.6	**94.4**	**17.50**
Tetrachlooretheen	0.10	569.1	163.7	138.3	**290.4**	**241.72**	2.00	165.6	172.6	157.8	**165.3**	**7.40**	10.00	159.4	150.9	224.7	**178.4**	**40.34**
Tetrachloormethaan	0.10	545.6	100.0	83.7	**243.1**	**262.09**	2.00	106.2	101.0	94.8	**100.6**	**5.71**	10.00	92.3	81.3	116.4	**96.7**	**17.95**
Tetradecaan	0.10	127.9	129.1	97.8	**118.3**	**17.73**	1.91	127.3	148.9	104.0	**126.7**	**22.48**	9.55	83.4	84.0	119.2	**95.6**	**20.50**
THF (tetrahydrofuran)	0.10	404.2	88.9	82.9	**192.0**	**183.77**	2.00	94.7	96.2	93.6	**94.8**	**1.29**	10.00	82.9	73.0	106.8	**87.6**	**17.36**
THT (tetrahydrothiofeen)	0.12	164.5	54.8	28.1	**82.5**	**72.31**	2.50	52.2	55.0	43.2	**50.1**	**6.15**	12.49	48.9	41.9	65.2	**52.0**	**11.94**
Tolueen	0.10	442.8	144.8	114.1	**233.9**	**181.57**	2.00	101.7	105.3	92.8	**99.9**	**6.47**	10.00	89.8	84.1	124.4	**99.4**	**21.82**
trans-1,2-Dichlooretheen	0.10	661.4	80.6	79.4	**273.8**	**335.67**	2.00	92.3	89.3	97.9	**93.2**	**4.36**	10.00	95.8	70.9	115.7	**94.1**	**22.44**
trans-1,3-Dichloorpropeen	0.10	302.1	96.9	74.3	**157.7**	**125.52**	2.00	101.0	99.5	89.9	**96.8**	**5.98**	10.00	82.5	75.9	108.9	**89.1**	**17.48**
trans-2-Methylcyclohexanol	0.12	57.7	93.9	57.6	**69.7**	**20.91**	2.31	37.4	33.9	24.0	**31.8**	**6.95**	11.55	58.0	59.8	76.8	**64.8**	**10.37**
trans-4-Methylcyclohexanol	0.11	-	-	-	-	-	2.29	13.7	14.8	8.5	**12.3**	**3.35**	11.43	45.3	46.6	55.8	**49.2**	**5.70**
trans-Decalin	0.11	256.5	96.5	71.5	**141.5**	**100.39**	2.24	103.8	115.4	96.1	**105.1**	**9.74**	11.20	87.7	86.1	117.4	**97.1**	**17.62**
Tribroommethaan	0.10	160.8	87.0	60.6	**102.8**	**51.92**	2.00	97.5	101.6	84.4	**94.5**	**9.01**	10.00	77.2	77.3	113.0	**89.1**	**20.67**
Trichlooretheen	0.10	521.5	100.3	86.5	**236.1**	**247.24**	2.00	110.5	109.7	105.2	**108.4**	**2.87**	10.00	98.9	91.5	133.2	**107.8**	**22.24**
Trichloormethaan	0.10	517.6	93.3	89.8	**233.6**	**245.95**	2.00	91.5	91.3	93.2	**92.0**	**1.05**	10.00	73.6	63.7	95.5	**77.6**	**16.27**
Trichloormonofluormethaan	0.10	647.3	137.2	131.7	**305.4**	**296.11**	2.00	91.4	110.6	97.4	**99.8**	**9.85**	10.00	57.7	45.0	82.1	**61.6**	**18.82**
Tridecaan	0.09	108.4	81.0	58.0	**82.5**	**25.24**	1.89	108.1	125.4	93.3	**109.0**	**16.03**	9.45	85.3	85.2	113.6	**94.7**	**16.34**
Undecaan	0.09	231.9	93.4	75.9	**133.8**	**85.44**	1.85	109.9	126.7	98.7	**111.8**	**14.06**	9.25	91.2	90.6	122.8	**101.5**	**18.42**
Vinylchloride	0.10	568.4	98.9	122.2	**263.2**	**264.63**	2.00	81.2	79.6	57.3	**72.7**	**13.37**	10.00	37.5	20.7	31.1	**29.8**	**8.44**

11 APPENDIX IV: RESULTS METHOD PERFORMANCE AND VALIDATION

Table 13. Raw data on linearity, measured on system 1. Linearity range measured was 0.1 – 10 mg/L.

Compounds	Internal standard	Lower (mg/L)	Upper (mg/L)	n	R^2
Vinylchloride	Vinylchloride-D3	0.1	5	6	0.9999
1,1-Dichloroethene	Benzene-D6	0.1	10	8	0.9992
Dichloromethane	Benzene-D6	0.1	10	8	0.9982
MTBE	Benzene-D6	0.1	10	8	0.9998
Acrylonitrile	Benzene-D6	0.1	7.5	7	0.9967
trans-1,2-Dichloroethene	Benzene-D6	0.1	10	8	0.9997
1,1-Dichloroethane	Benzene-D6	0.1	10	8	0.9997
ETBE	Benzene-D6	0.1	10	8	0.9999
cis-1,2-Dichloroethene	Benzene-D6	0.1	10	8	0.9999
Trichloromethane	Benzene-D6	0.1	10	8	0.9999
1,1,1-Trichloroethane	Benzene-D6	0.1	10	8	0.9998
Tetrachloromethane	Benzene-D6	0.1	10	8	0.9989
Benzene	Benzene-D6	0.1	10	8	0.9994
1,2-Dichloroethane	Benzene-D6	0.1	10	8	0.9999
1,1-Dichloropropane	Benzene-D6	0.1	10	8	0.9998
Trichloroethene	Benzene-D6	0.1	10	8	0.9995
1,2-Dichloropropane	Benzene-D6	0.1	10	8	0.9999
Toluene	Benzene-D6	0.1	10	8	0.9993
1,1,2-Trichloroethane	Benzene-D6	0.1	10	8	0.9998
Tetrachloroethene	Benzene-D6	0.1	10	8	0.9990
1,3-Dichlorpropane	Benzene-D6	0.1	10	8	0.9998
Monochlorobenzene	Benzene-D6	0.1	10	8	0.9995
Ethylbenzene	Benzene-D6	0.1	10	8	0.9993
p,m-Xylene	Benzene-D6	0.1	10	8	0.9992
o-Xylene	Benzene-D6	0.1	10	8	0.9993
Styrene	Benzene-D6	0.1	10	8	0.9989
Tribromomethane	Benzene-D6	0.1	10	8	0.9976
Cumene	Benzene-D6	0.1	10	8	0.9992
1,2,3-Trichloropropane	Benzene-D6	0.1	10	8	0.9993
1,3-Dichlorobenzene	Benzene-D6	0.1	10	8	0.9994
1,4-Dichlorobenzene	Benzene-D6	0.1	10	8	0.9993
1,2-Dichlorobenzene	Benzene-D6	0.1	10	8	0.9995
1,3,5-Trichlorobenzene	Benzene-D6	0.1	10	8	0.9992
1,2,4-Trichlorobenzene	Benzene-D6	0.1	10	8	0.9992
Naphthalene	Naphthalene-D3	0.1	10	8	0.9992
1,2,3-Trichlorobenzene	Benzene-D6	0.1	10	8	0.9991
Dichlorodifluoromethane	Vinylchloride-D3	0.1	7.5	7	0.9955
Chloromethane	Vinylchloride-D3	0.1	7.5	7	0.9986
Bromomethane	Vinylchloride-D3	0.1	10	8	0.9995
Chloroethane	Vinylchloride-D3	0.1	10	8	0.9983
Trichloromonofluoromethane	Benzene-D6	0.1	10	8	0.9982
Ethylether	Benzene-D6	0.1	10	8	0.9990
1,1,2-Trichloro-1,2,2-trifluoroethane	Benzene-D6	0.1	10	8	0.9987
Iodomethane	Benzene-D6	0.1	10	8	0.9999
n-Hexane	Benzene-D6	0.1	10	8	0.9998
Diisopropylether	Benzene-D6	0.1	10	8	0.9999
2-Chloro-1,3-butadiene	Benzene-D6	0.1	10	8	0.9998
2,2-Dichloropropane	Benzene-D6	0.1	10	8	0.9998
Methacrylonitrile	Benzene-D6	0.1	10	8	0.9991
THF (tetrahydrofuran)	Benzene-D6	0.1	10	8	0.9998
Bromochloromethane	Benzene-D6	0.1	10	8	0.9999
1,1-Dichloropropene	Benzene-D6	0.1	10	8	0.9997
TAME	Benzene-D6	0.1	10	8	0.9998
n-Heptane	Benzene-D6	0.1	10	8	0.9993
2,3-Dichloropropene	Benzene-D6	0.1	10	8	0.9994
Methylmethacrylate	Benzene-D6	0.1	10	8	0.9994
Dibromomethane	Benzene-D6	0.1	10	8	0.9995

(Table 13 continuing)

Compounds	Internal standard	Lower (mg/L)	Upper (mg/L)	n	R^2
Bromodichloromethane	Benzene-D6	0.1	10	8	0.9997
cis-1,3-Dichloropropene	Benzene-D6	0.1	10	8	0.9996
n-Octane	Benzene-D6	0.1	10	8	0.9990
trans-1,3-Dichloropropene	Benzene-D6	0.1	10	8	0.9995
Ethylmethacrylate	Benzene-D6	0.1	10	8	0.9986
Dibromochloromethane	Benzene-D6	0.1	10	8	0.9988
1,2-Dibromoethane	Benzene-D6	0.1	10	8	0.9993
1,1,1,2-Tetrachloroethane	Benzene-D6	0.1	10	8	0.9991
n-Nonane	Benzene-D6	0.1	10	8	0.9994
3-Ethyltoluene	Benzene-D6	0.1	10	8	0.9992
1,1,2,2-Tetrachloroethane	Benzene-D6	0.1	10	8	0.9991
Bromobenzene	Benzene-D6	0.1	10	8	0.9991
Propylbenzene	Benzene-D6	0.1	10	8	0.9991
2-Chlorotoluene	Benzene-D6	0.1	10	8	0.9995
4-Ethyltoluene	Benzene-D6	0.1	10	8	0.9991
1,3,5-Trimethylbenzene	Benzene-D6	0.1	10	8	0.9992
n-Decane	Benzene-D6	0.1	10	8	0.9993
4-Chlorotoluene	Benzene-D6	0.1	10	8	0.9993
2-Ethyltoluene	Benzene-D6	0.1	10	8	0.9992
tert-Butylbenzene	Benzene-D6	0.1	10	8	0.9992
Pentachloroethane	Benzene-D6	0.1	10	8	0.9985
1,2,4-Trimethylbenzene	Benzene-D6	0.1	10	8	0.9992
sec-Butylbenzene	Benzene-D6	0.1	10	8	0.9992
p-Isopropyltoluene	Benzene-D6	0.1	10	8	0.9991
1,2,3-Trimethylbenzene	Benzene-D6	0.1	10	8	0.9990
Butylbenzene	Benzene-D6	0.1	10	8	0.9992
Hexachloroethane	Benzene-D6	0.1	10	8	0.9995
1,2-Dibromo-3-chloropropane	Benzene-D6	0.1	10	8	0.9982
Hexachlorobutadiene	Benzene-D6	0.1	10	8	0.9989
1,3-Butadiene	Vinylchloride-D3	0.1	10	8	0.9982
2-Methylbutane	Vinylchloride-D3	0.1	10	8	0.9991
2,2-Dimethylbutane	Benzene-D6	0.1	10	8	0.9997
Cyclopentane	Benzene-D6	0.1	10	8	0.9988
2,4-Dimethylpentane	Benzene-D6	0.1	10	8	0.9997
Methyl acrylate	Benzene-D6	0.1	10	8	0.9998
Cyclohexane	Benzene-D6	0.1	10	8	0.9992
2-Methoxyethanol (methyl cellosolve)	Benzene-D6	0.1	10	8	0.9985
2-Methyl-2-butanol	Benzene-D6	0.1	7.5	7	0.9987
3-Methyl-2-butanone	Benzene-D6	0.1	10	8	0.9996
PGME	Benzene-D6	0.1	7.5	7	0.9940
Methyl propyl ketone	Benzene-D6	0.1	10	8	0.9996
Ethyl propionate	Benzene-D6	0.1	10	8	0.9993
1,4-Dioxane	Benzene-D6	0.1	10	8	0.9998
Ethylene chlorohydrin	Benzene-D6	0.1	7.5	7	0.9984
3-Pentanol	Benzene-D6	0.1	7.5	7	0.9982
EPI	Benzene-D6	0.1	10	8	0.9997
3-methyl-1-Butanol	Benzene-D6	0.1	7.5	7	0.9972
Methyl isobutyl carbinol	Benzene-D6	0.1	7.5	7	0.9973
Isopropyl glycol	Benzene-D6	0.1	7.5	7	0.9951
Ethylene glycol diethyl ether	Benzene-D6	0.1	10	8	0.9993
2,4-Dimethyl-3-pentanone	Benzene-D6	0.1	10	8	0.9994
n-Butylacetate	Benzene-D6	0.1	10	8	0.9994
THT	Benzene-D6	0.1	10	8	0.9992
2-Propoxyethanol	Benzene-D6	0.5	10	6	0.9959
Dimethyl formamide	Benzene-D6	5	10	3	0.9781
Isopropyl glycidil ether	Benzene-D6	0.1	10	8	0.9988
Isopentyl acetate	Benzene-D6	0.1	10	8	0.9994
4-Hydroxy-4-methyl-2-pentanone	Benzene-D6	0.1	7.5	7	0.9969
1-Bromo-3-chloropropane	Benzene-D6	0.1	10	8	0.9994

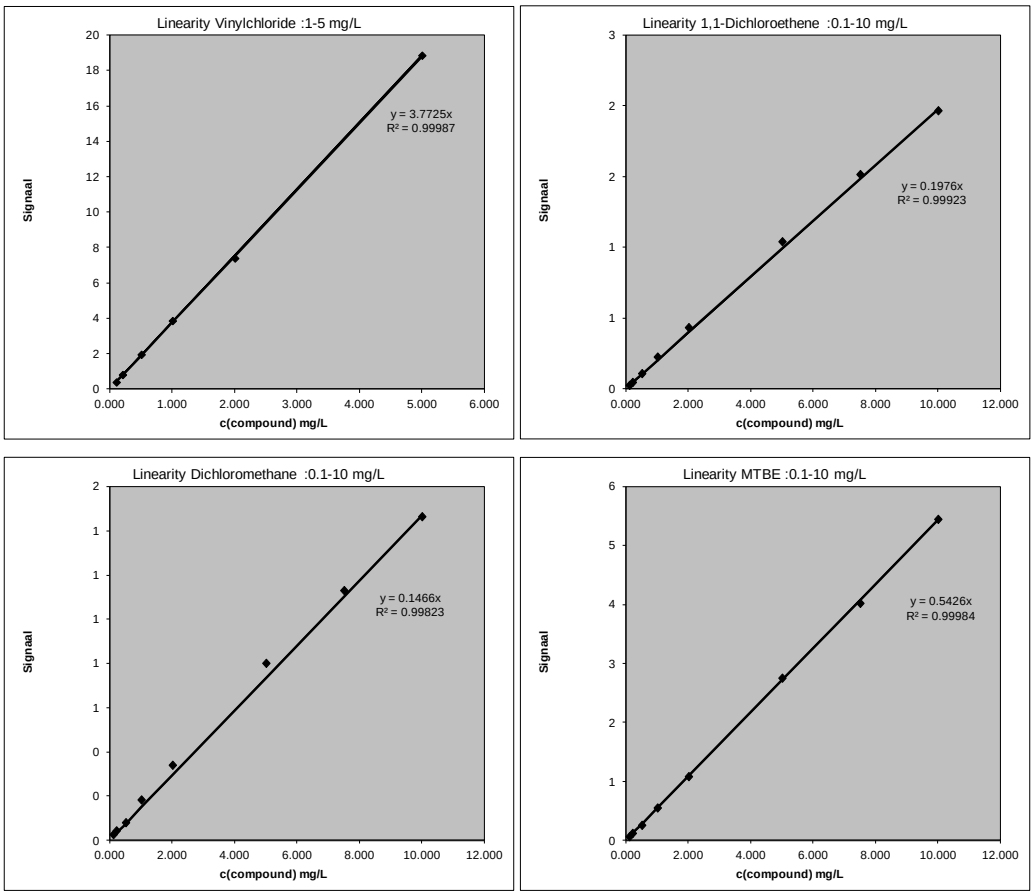
(Table 13 continuing)

Compounds	Internal standard	Lower (mg/L)	Upper (mg/L)	n	R^2
Furfuryl alcohol	Benzene-D6	0.5	7.5	5	0.9976
Butylpropionate	Benzene-D6	0.1	10	8	0.9994
2-Ethoxyethyl acetate	Benzene-D6	0.2	10	7	0.9991
Cyclohexanol	Benzene-D6	0.1	10	8	0.9951
a-Pinene	Benzene-D6	0.1	10	8	0.9988
Cyclohexanone	Benzene-D6	0.1	10	8	0.9986
5-methyl-3-heptanone	Benzene-D6	0.1	10	8	0.9984
trans-2-Methylcyclohexanol	Benzene-D6	0.2	7.5	6	0.9965
Butylmethacrylate	Benzene-D6	0.1	10	8	0.9978
cis-4-Methylcyclohexanol	Benzene-D6	0.1	10	8	0.9959
trans-4-Methylcyclohexanol	Benzene-D6	0.2	7.5	6	0.9971
2-Methylcyclohexanone	Benzene-D6	0.1	10	8	0.9988
3-Methylcyclohexanone	Benzene-D6	0.1	10	8	0.9985
4-Methylcyclohexanone	Benzene-D6	0.1	10	8	0.9981
Isobutyl benzene	Benzene-D6	0.1	10	8	0.9992
D-Limonene	Benzene-D6	0.1	10	8	0.9975
Benzyl chloride	Benzene-D6	0.1	10	8	0.9978
1,4-Diethylbenzene	Benzene-D6	0.1	10	8	0.9987
Diethylene glycol diethyl ether	Benzene-D6	0.5	10	6	0.9977
Benzyl alcohol	Benzene-D6	0.5	7.5	5	0.9957
1-Methyl-2-pyrrolidon	Benzene-D6	2	10	4	0.9947
cis-Decalin	Benzene-D6	0.1	10	8	0.9987
1,4-Diisopropylbenzene	Benzene-D6	0.1	10	8	0.9985
Isophoron	Naphthalene-D8	0.1	10	8	0.9950
Benzyl acetate	Naphthalene-D8	0.1	10	8	0.9989
1,3-Diisopropylbenzene	Naphthalene-D8	0.1	10	8	0.9901
n-Pentane	Benzene-D6	0.1	10	8	0.0318
Ethanol	Benzene-D6	0.1	7.5	7	0.9955
Methylal	Benzene-D6	0.1	10	8	0.9989
Aceton	Benzene-D6	0.1	10	8	0.9909
2-Methylpentane	Benzene-D6	0.1	10	8	0.9984
tert-Butanol	Benzene-D6	0.1	7.5	7	0.9955
Allyl alcohol	Benzene-D6	0.1	7.5	7	0.9963
n-Propanol	Benzene-D6	0.1	7.5	7	0.9973
Methylcyclopentane	Benzene-D6	0.1	10	8	0.9996
MEK (2-Butanone)	Benzene-D6	0.1	10	8	0.9981
Ethyl acetate	Benzene-D6	0.1	10	8	0.9999
2-Butanol	Benzene-D6	0.1	7.5	7	0.9982
2-Methyl-1-propanol	Benzene-D6	0.1	7.5	7	0.9982
Ethylene glycol dimethyl ether	Benzene-D6	0.1	10	8	0.9985
Isopropyl acetate	Benzene-D6	0.1	10	8	0.9997
Cyclohexene	Benzene-D6	0.1	10	8	0.9966
1-Butanol	Benzene-D6	0.1	7.5	7	0.9974
Ethylacrylate	Benzene-D6	0.1	10	8	0.9996
Methylcyclohexane	Benzene-D6	0.1	10	8	0.9992
3-Pentanone	Benzene-D6	0.1	10	8	0.9995
n-Propyl acetate	Benzene-D6	0.1	10	8	0.9998
2-Pentanol	Benzene-D6	0.1	7.5	7	0.9979
2-Ethoxyethanol	Benzene-D6	0.5	7.5	5	0.9978
Methyl isobutyl ketone	Benzene-D6	0.1	10	8	0.9994
Isobutyl acetate	Benzene-D6	0.1	10	8	0.9994
1-Pentanol	Benzene-D6	0.2	7.5	6	0.9976
Methyl-n-butyl ketone	Benzene-D6	0.1	10	8	0.9991
Mesityl oxide	Benzene-D6	0.1	10	8	0.9983
Cyclopentanone	Benzene-D6	0.1	10	8	0.9992
4-Vinyl-1-cyclohexene	Benzene-D6	0.1	10	8	0.9988
Ethylene glycol methylether acetate	Benzene-D6	0.1	10	8	0.9988
Dibutyl ether	Benzene-D6	0.1	10	8	0.9989
PGMEA	Benzene-D6	0.1	10	8	0.9990

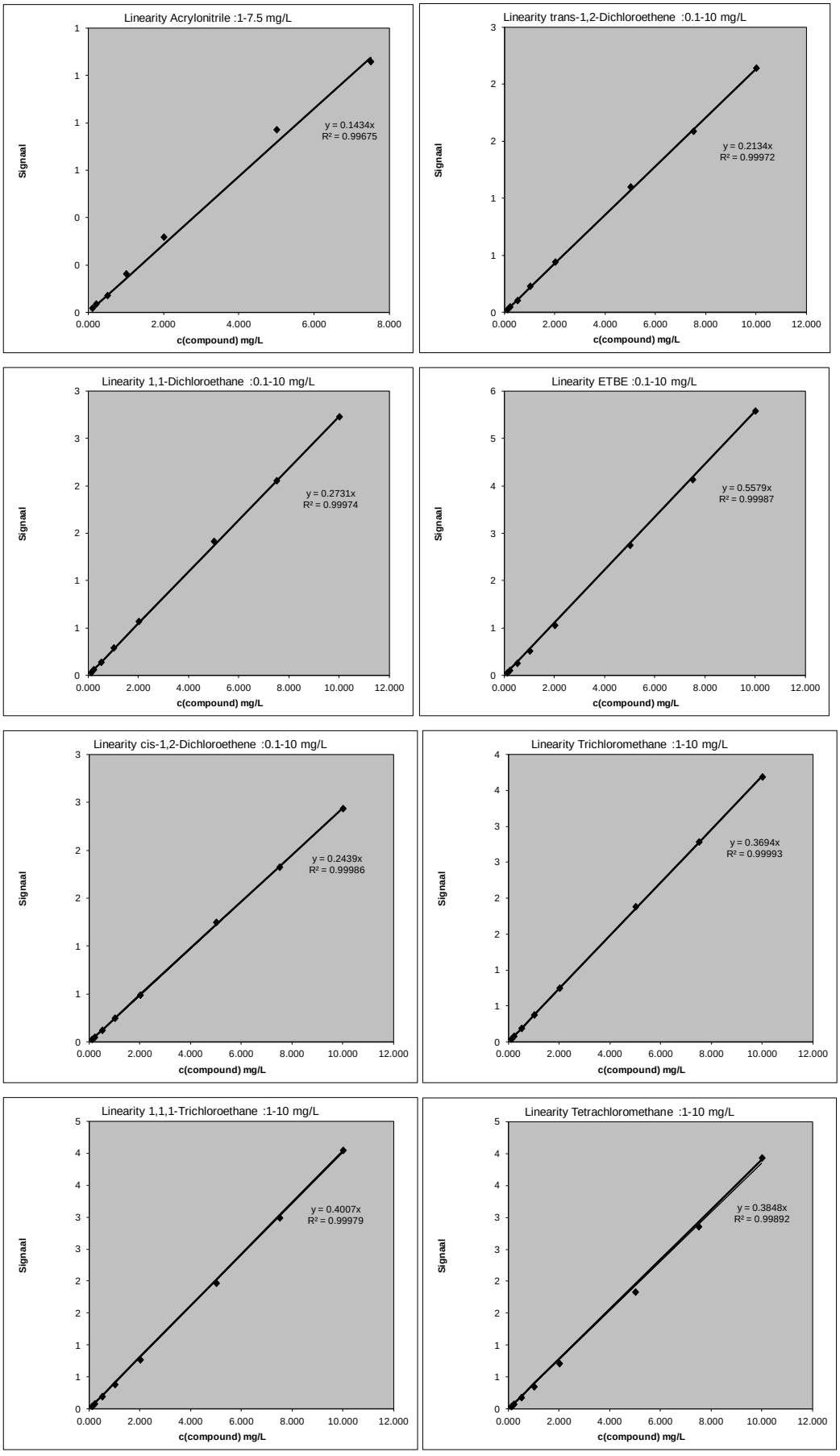
(Table 13 continuing)

Compounds	Internal standard	Lower (mg/L)	Upper (mg/L)	n	R^2
Furfural	Benzene-D6	0.2	10	7	0.9974
Methyl isoamyl ketone	Benzene-D6	0.1	10	8	0.9987
4-Heptanone	Benzene-D6	0.1	10	8	0.9990
Butylacrylate	Benzene-D6	0.1	10	8	0.9986
3-Heptanone	Benzene-D6	0.1	10	8	0.9989
Methyl amyl ketone	Benzene-D6	0.1	10	8	0.9975
n-Amyl acetate	Benzene-D6	0.1	10	8	0.9991
n,n-Dimethylacetamide	Benzene-D6	0.5	7.5	5	0.9888
Ethylene glycol monobutyl ether	Benzene-D6	0.5	10	6	0.9942
cis-2-Methylcyclohexanol	Benzene-D6	0.2	7.5	6	0.9972
Diisobutyl ketone	Benzene-D6	0.1	10	8	0.9987
a-Methylstyrene	Benzene-D6	0.1	10	8	0.9985
Butyl glycidil ether	Benzene-D6	0.2	10	7	0.9987
Ethylene glycoldiacetate	Benzene-D6	0.2	7.5	6	0.9977
Dichloroethyl ether	Benzene-D6	0.1	10	8	0.9990
Dipropyleneglycol methyl ether	Benzene-D6	0.1	10	8	0.9980
1,3-Diethylbenzene	Benzene-D6	0.1	10	8	0.9988
trans-Decalin	Naphthalene-D8	0.1	10	8	0.9991
1,2-Diethylbenzene	Naphthalene-D8	0.1	10	8	0.9992
Undecane	Naphthalene-D8	0.1	10	8	0.9988
2-Butoxy ethyl acetate	Naphthalene-D8	0.1	10	8	0.9989
tert-Butyltoluene	Naphthalene-D8	0.1	10	8	0.9990
Dodecane	Naphthalene-D8	0.1	10	8	0.9985
1,2,3,4-Tetrahydronaftalene	Naphthalene-D8	0.1	10	8	0.9987
Tridecane	Naphthalene-D8	0.1	10	8	0.9981
Tetradecane	Naphthalene-D8	0.1	10	8	0.9972
Pentadecane	Naphthalene-D8	0.1	10	8	0.9963
Hexadecane	Naphthalene-D8	0.1	10	8	0.9955

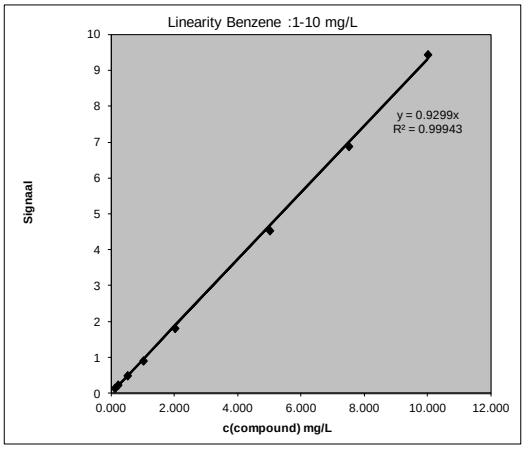
(Figure 2)

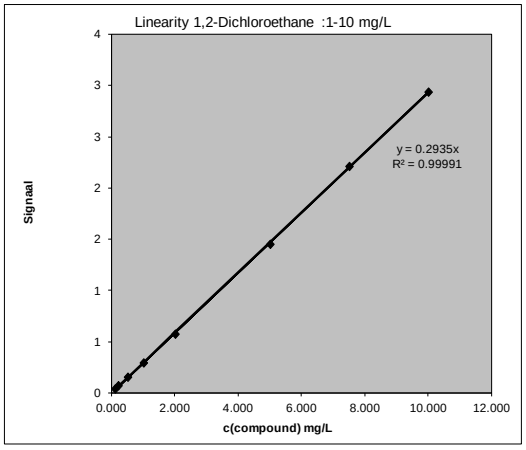


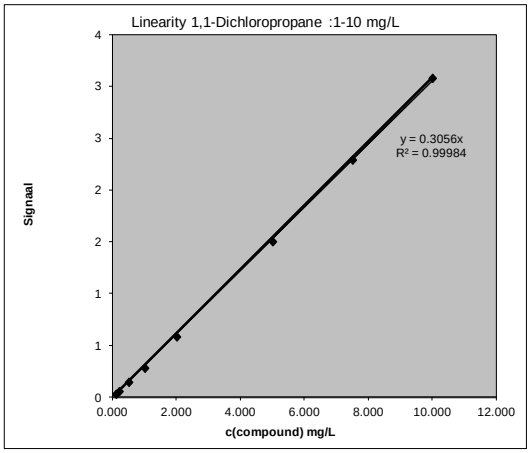
(Figure 2)

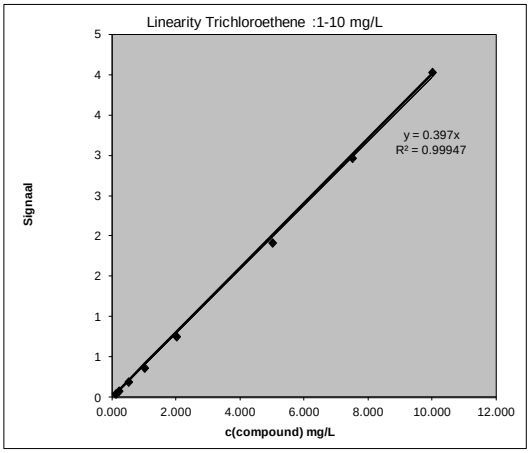

Linearity Acrylonitrile :1-7.5 mg/L
y = 0.1434x
R² = 0.99675
Signaal
c(compound) mg/L
Linearity trans-1,2-Dichloroethene :0.1-10 mg/L
y = 0.2134x
R² = 0.99972
Signaal
c(compound) mg/L
Linearity 1,1-Dichloroethane :0.1-10 mg/L
y = 0.2731x
R² = 0.99974
Signaal
c(compound) mg/L
Linearity ETBE :0.1-10 mg/L
y = 0.5579x
R² = 0.99987
Signaal
c(compound) mg/L
Linearity cis-1,2-Dichloroethene :0.1-10 mg/L
y = 0.2439x
R² = 0.99986
Signaal
c(compound) mg/L
Linearity Trichloromethane :1-10 mg/L
y = 0.3694x
R² = 0.99993
Signaal
c(compound) mg/L
Linearity 1,1,1-Trichloroethane :1-10 mg/L
y = 0.4007x
R² = 0.99979
Signaal
c(compound) mg/L
Linearity Tetrachloromethane :1-10 mg/L
y = 0.3848x
R² = 0.99892
Signaal
c(compound) mg/L

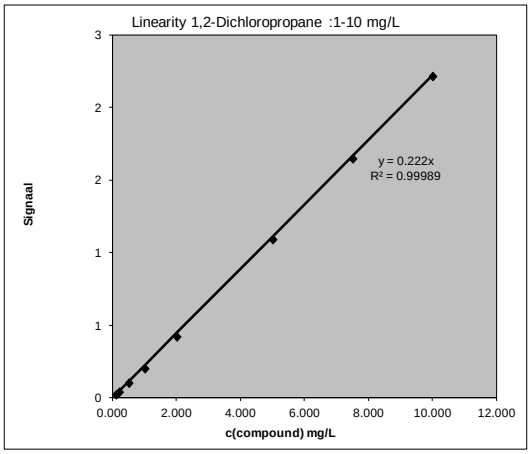
(Figure 2)

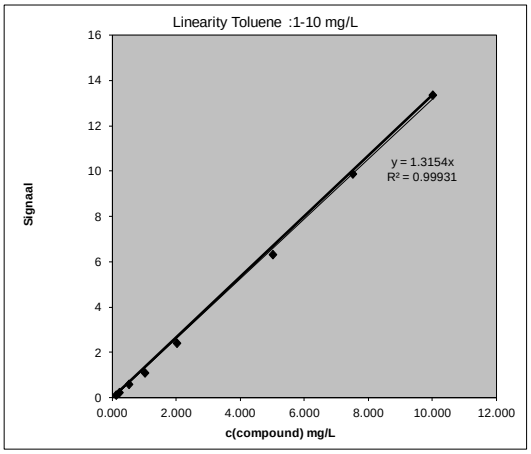

Linearity Benzene :1-10 mg/L
y = 0.9299x
R² = 0.99943
Signaal
c(compound) mg/L

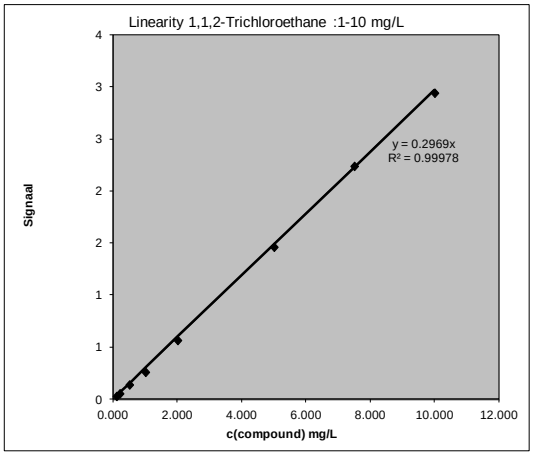

Linearity 1,2-Dichloroethane :1-10 mg/L
y = 0.2935x
R² = 0.99991
Signaal
c(compound) mg/L

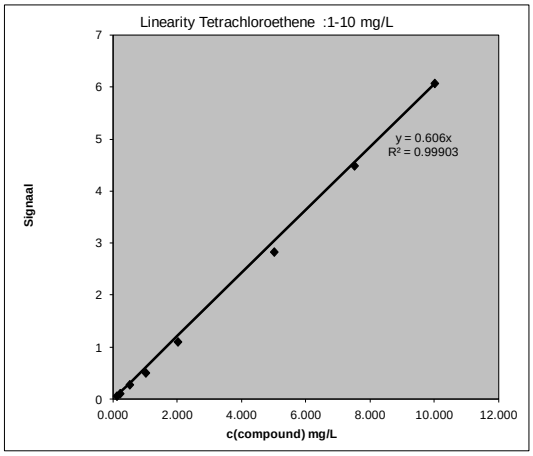

Linearity 1,1-Dichloropropane :1-10 mg/L
y = 0.3056x
R² = 0.99984
Signaal
c(compound) mg/L


Linearity Trichloroethene :1-10 mg/L
y = 0.397x
R² = 0.99947
Signaal
c(compound) mg/L

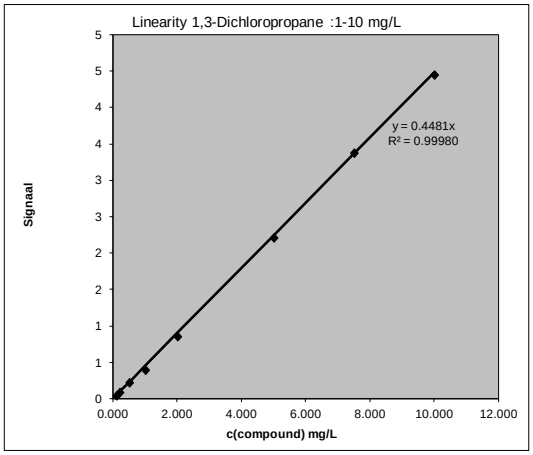

Linearity 1,2-Dichloropropane :1-10 mg/L
y = 0.222x
R² = 0.99989
Signaal
c(compound) mg/L

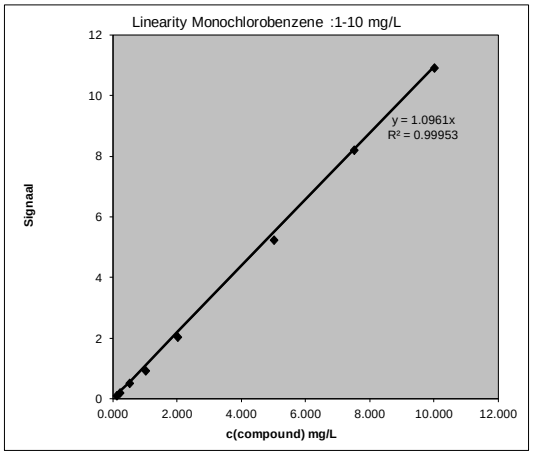

Linearity Toluene :1-10 mg/L
y = 1.3154x
R² = 0.99931
Signaal
c(compound) mg/L

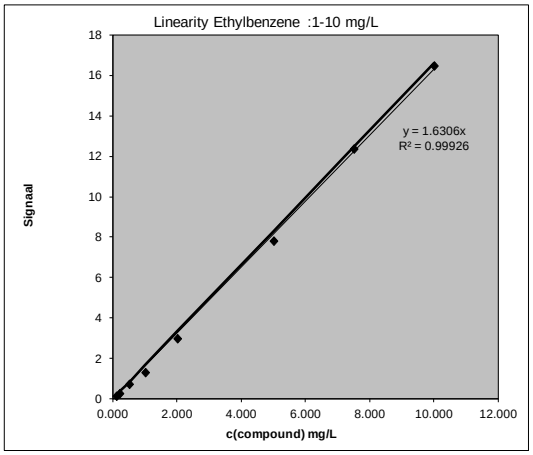

Linearity 1,1,2-Trichloroethane :1-10 mg/L
y = 0.2969x
R² = 0.99978
Signaal
c(compound) mg/L

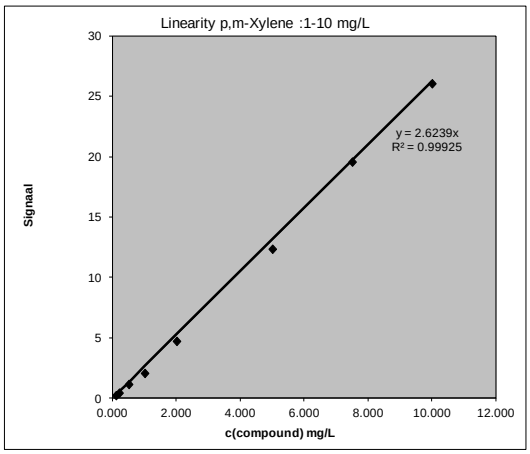

Linearity Tetrachloroethene :1-10 mg/L
y = 0.606x
R² = 0.99903
Signaal
c(compound) mg/L

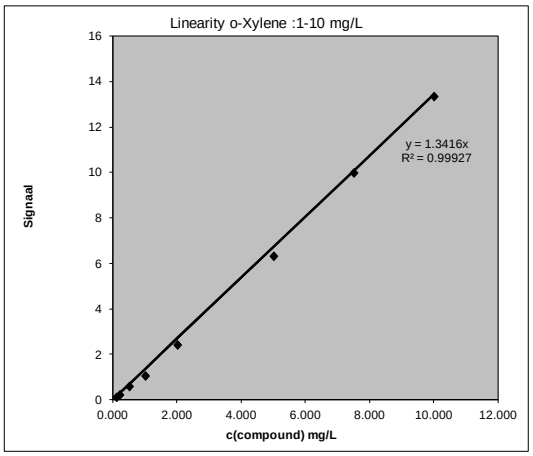
(Figure 2)

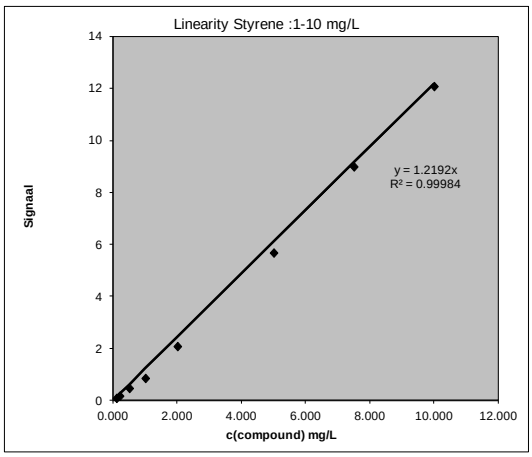

Linearity 1,3-Dichloropropane :1-10 mg/L
y = 0.4481x
R² = 0.99980
Signaal
c(compound) mg/L

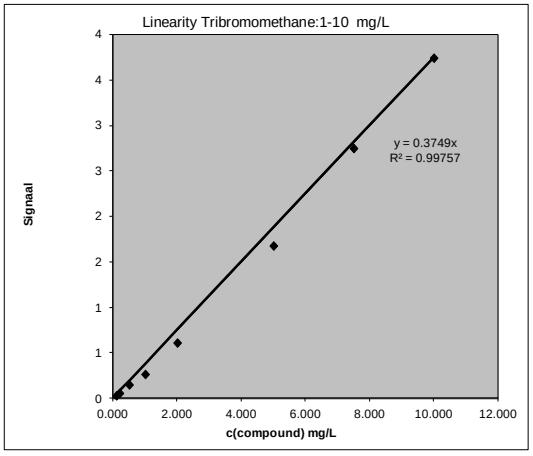

Linearity Monochlorobenzene :1-10 mg/L
y = 1.0961x
R² = 0.99953
Signaal
c(compound) mg/L

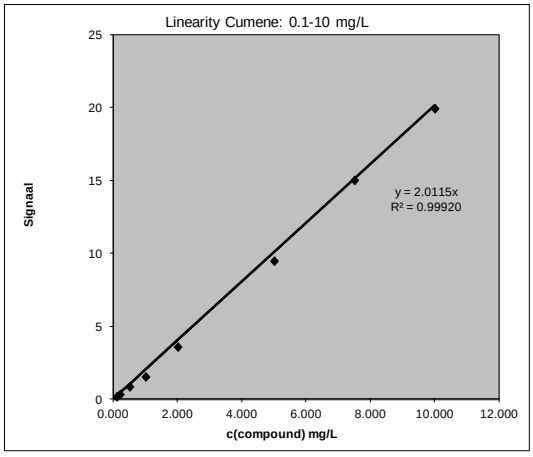

Linearity Ethylbenzene :1-10 mg/L
y = 1.6306x
R² = 0.99926
Signaal
c(compound) mg/L


Linearity p,m-Xylene :1-10 mg/L
y = 2.6239x
R² = 0.99925
Signaal
c(compound) mg/L

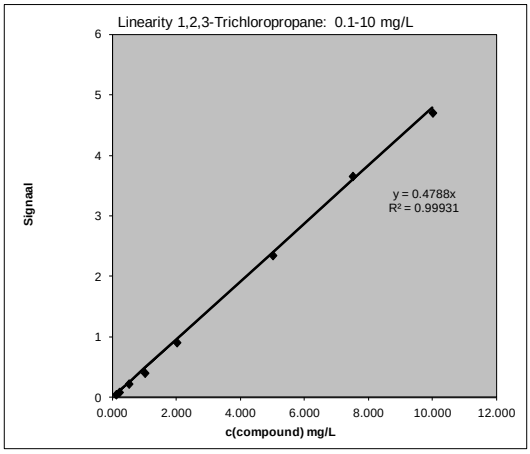

Linearity o-Xylene :1-10 mg/L
y = 1.3416x
R² = 0.99927
Signaal
c(compound) mg/L

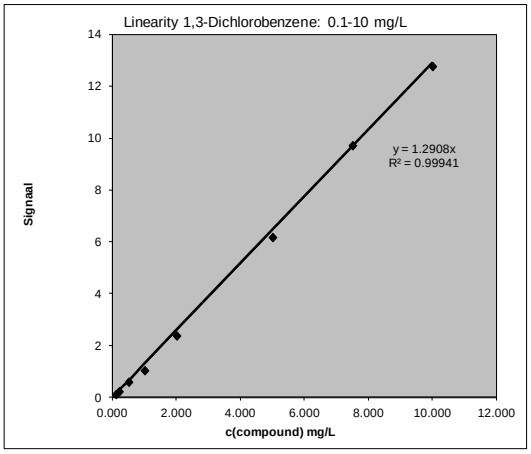

Linearity Styrene :1-10 mg/L
y = 1.2192x
R² = 0.99984
Signaal
c(compound) mg/L

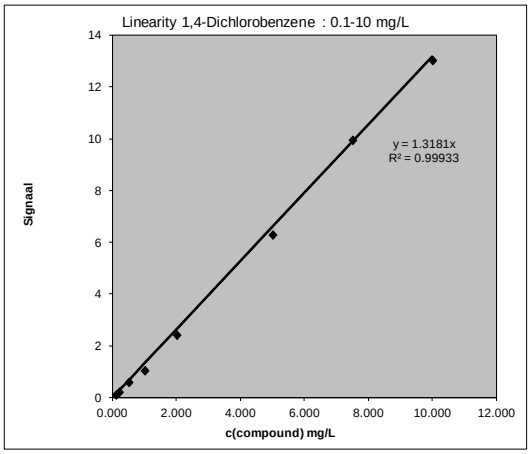

Linearity Tribromomethane:1-10 mg/L
y = 0.3749x
R² = 0.99757
Signaal
c(compound) mg/L

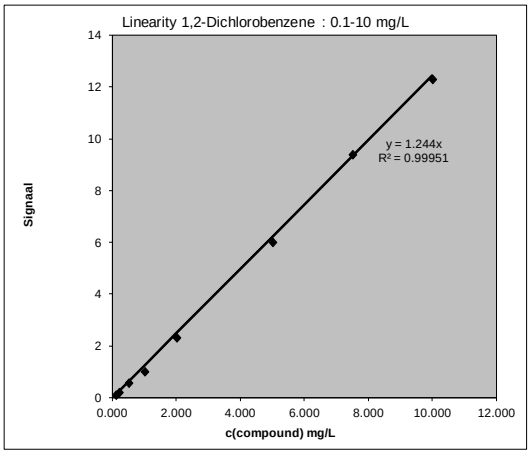

Linearity Cumene: 0.1-10 mg/L
y = 2.0115x
R² = 0.99920
Signaal
c(compound) mg/L

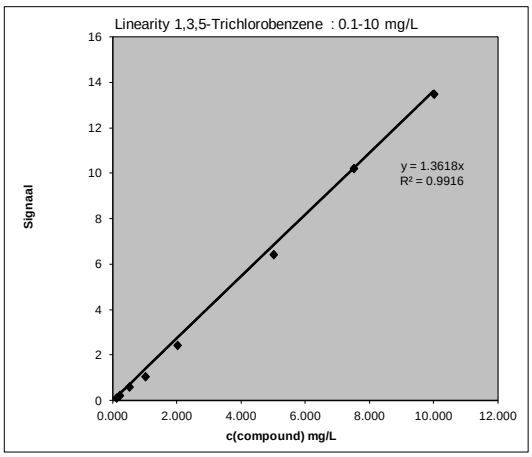
(Figure 2)

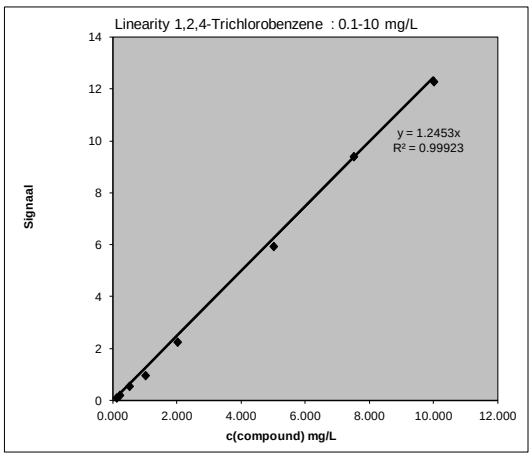

Linearity 1,2,3-Trichloropropane: 0.1-10 mg/L
y = 0.4788x
R² = 0.99931
Signaal
c(compound) mg/L

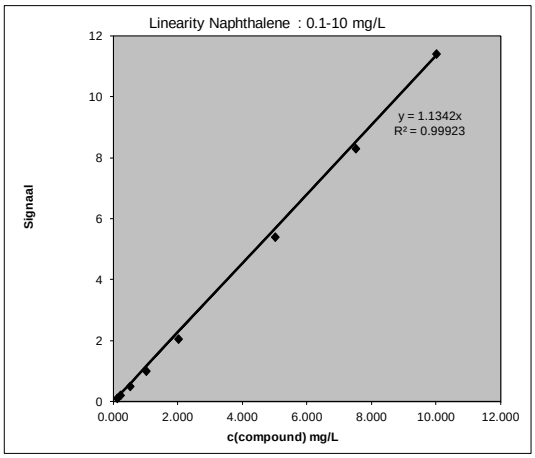

Linearity 1,3-Dichlorobenzene: 0.1-10 mg/L
y = 1.2908x
R² = 0.99941
Signaal
c(compound) mg/L

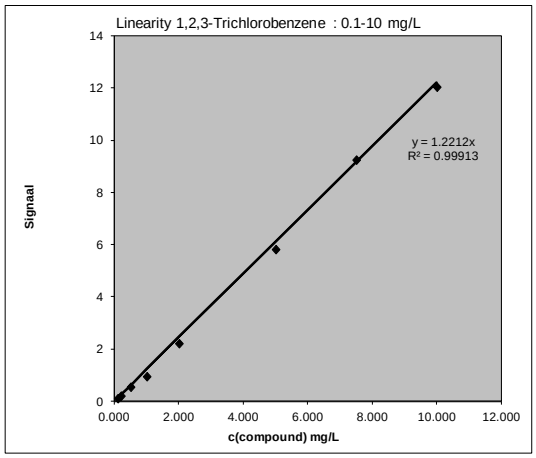

Linearity 1,4-Dichlorobenzene : 0.1-10 mg/L
y = 1.3181x
R² = 0.99933
Signaal
c(compound) mg/L


Linearity 1,2-Dichlorobenzene : 0.1-10 mg/L
y = 1.244x
R² = 0.99951
Signaal
c(compound) mg/L

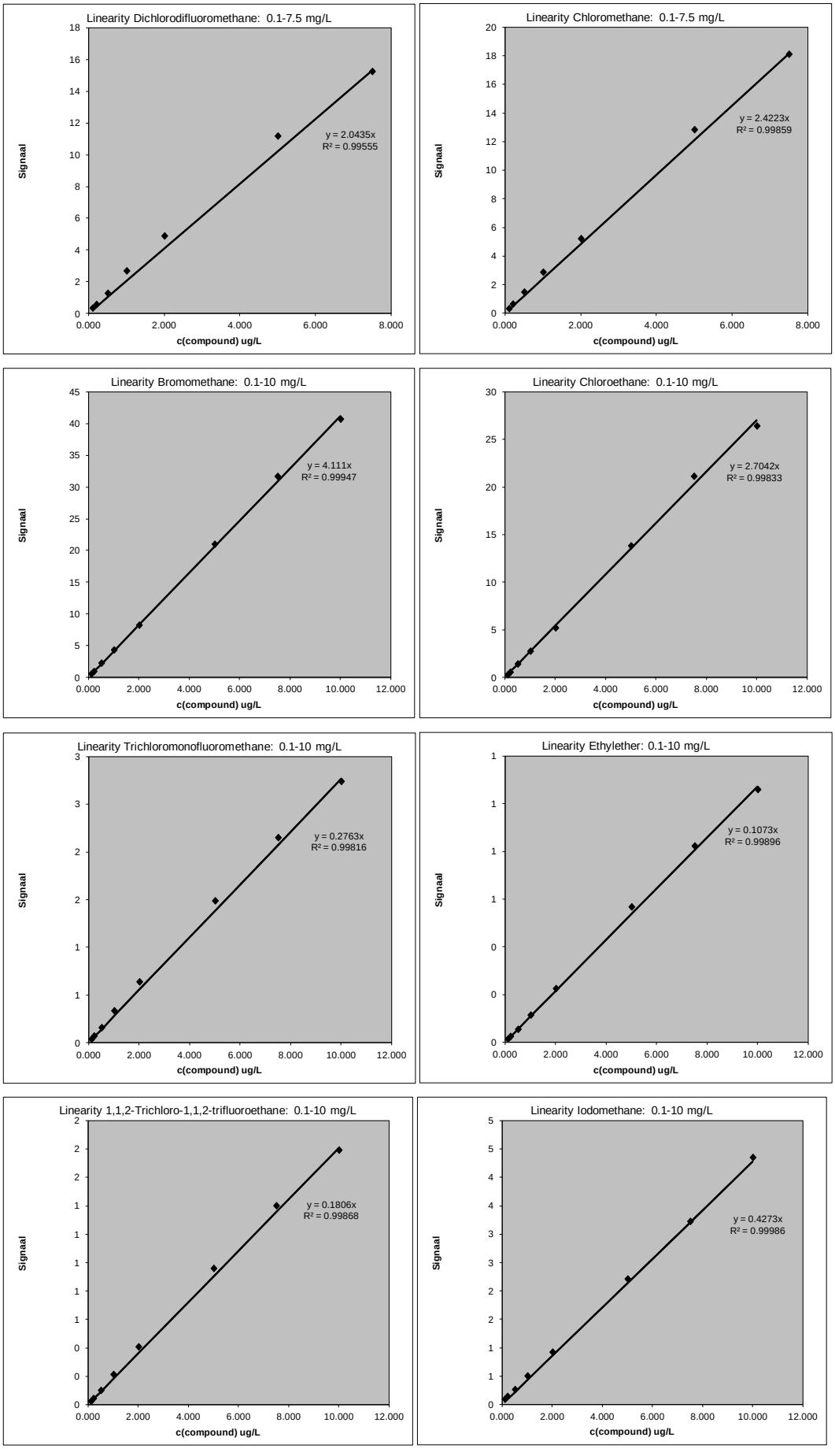

Linearity 1,3,5-Trichlorobenzene : 0.1-10 mg/L
y = 1.3618x
R² = 0.9916
Signaal
c(compound) mg/L


Linearity 1,2,4-Trichlorobenzene : 0.1-10 mg/L
y = 1.2453x
R² = 0.99923
Signaal
c(compound) mg/L

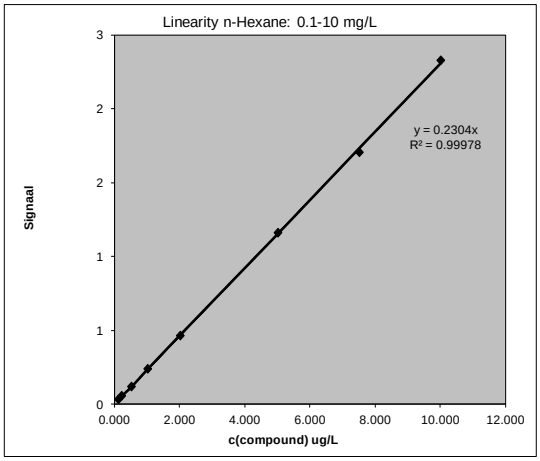

Linearity Naphthalene : 0.1-10 mg/L
y = 1.1342x
R² = 0.99923
Signaal
c(compound) mg/L

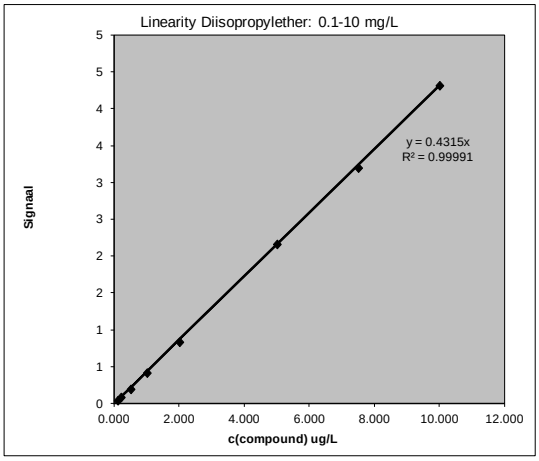

Linearity 1,2,3-Trichlorobenzene : 0.1-10 mg/L
y = 1.2212x
R² = 0.99913
Signaal
c(compound) mg/L

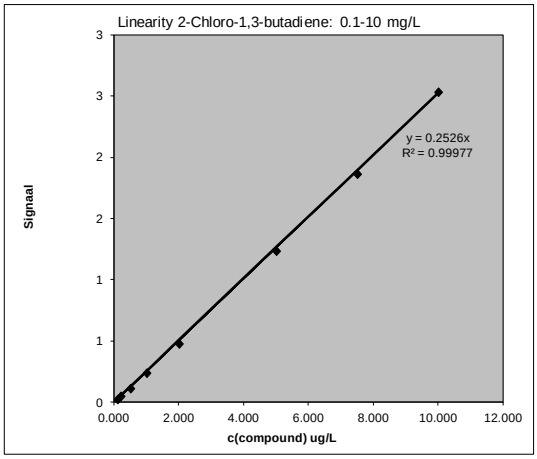
(Figure 2)

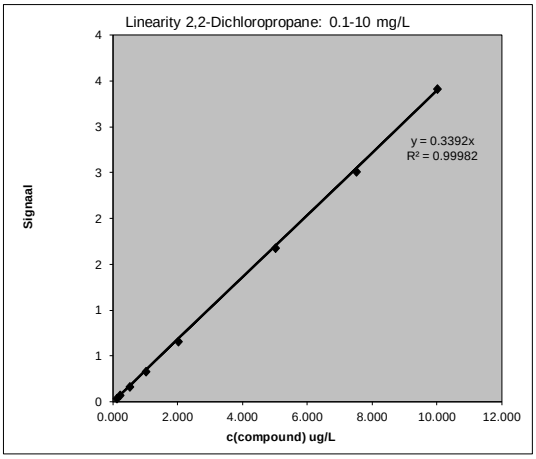

Linearity Dichlorodifluoromethane: 0.1-7.5 mg/L
y = 2.0435x
R² = 0.99555
Linearity Chloromethane: 0.1-7.5 mg/L
y = 2.4223x
R² = 0.99859
Linearity Bromomethane: 0.1-10 mg/L
y = 4.111x
R² = 0.99947
Linearity Chloroethane: 0.1-10 mg/L
y = 2.7042x
R² = 0.99833
Linearity Trichloromonofluoromethane: 0.1-10 mg/L
y = 0.2763x
R² = 0.99816
Linearity Ethylether: 0.1-10 mg/L
y = 0.1073x
R² = 0.99896
Linearity 1,1,2-Trichloro-1,1,2-trifluoroethane: 0.1-10 mg/L
y = 0.1806x
R² = 0.99868
Linearity Iodomethane: 0.1-10 mg/L
y = 0.4273x
R² = 0.99986
Signaal
c(compound) ug/L

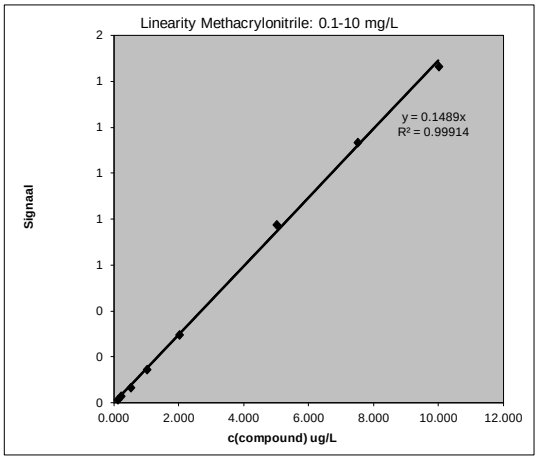
(Figure 2)

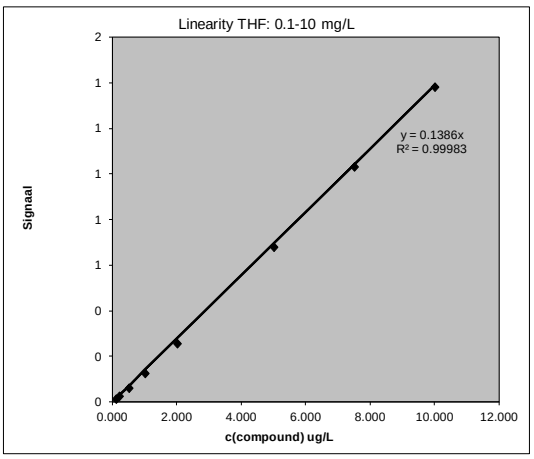

Linearity n-Hexane: 0.1-10 mg/L
y = 0.2304x
R² = 0.99978
Signaal
c(compound) ug/L

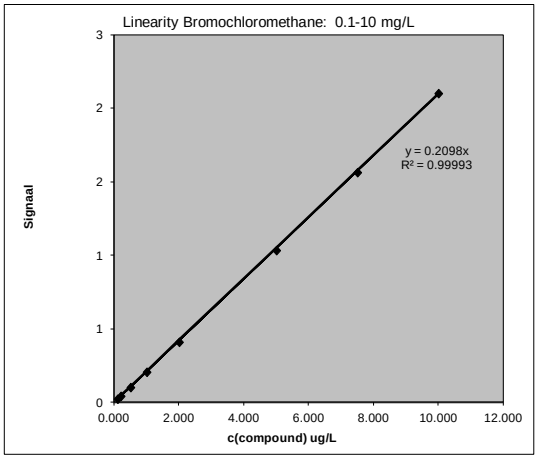

Linearity Diisopropylether: 0.1-10 mg/L
y = 0.4315x
R² = 0.99991
Signaal
c(compound) ug/L

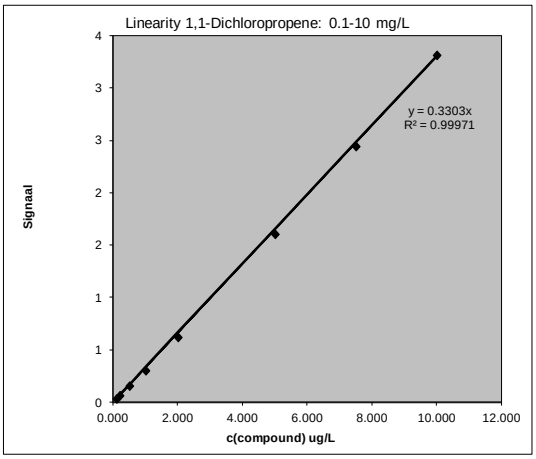

Linearity 2-Chloro-1,3-butadiene: 0.1-10 mg/L
y = 0.2526x
R² = 0.99977
Signaal
c(compound) ug/L


Linearity 2,2-Dichloropropane: 0.1-10 mg/L
y = 0.3392x
R² = 0.99982
Signaal
c(compound) ug/L

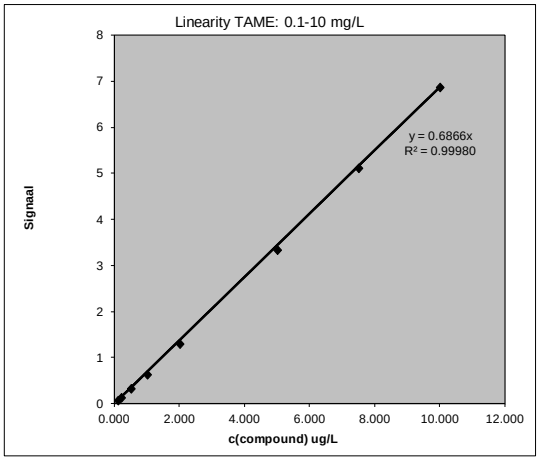

Linearity Methacrylonitrile: 0.1-10 mg/L
y = 0.1489x
R² = 0.99914
Signaal
c(compound) ug/L

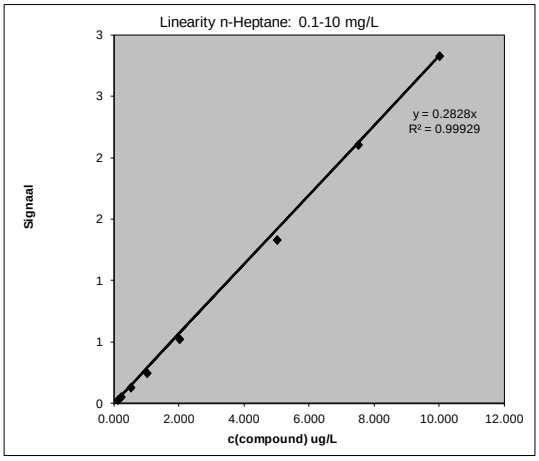

Linearity THF: 0.1-10 mg/L
y = 0.1386x
R² = 0.99983
Signaal
c(compound) ug/L

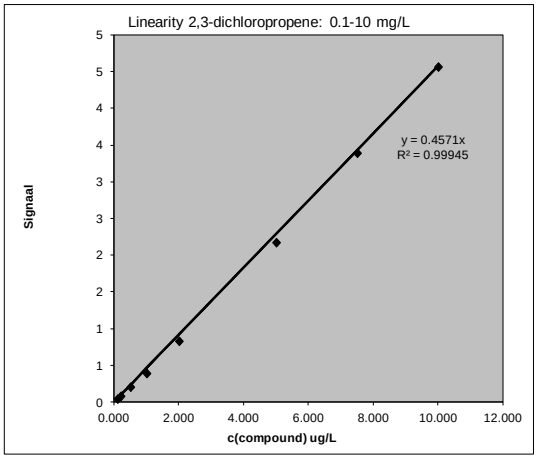

Linearity Bromochloromethane: 0.1-10 mg/L
y = 0.2098x
R² = 0.99993
Signaal
c(compound) ug/L

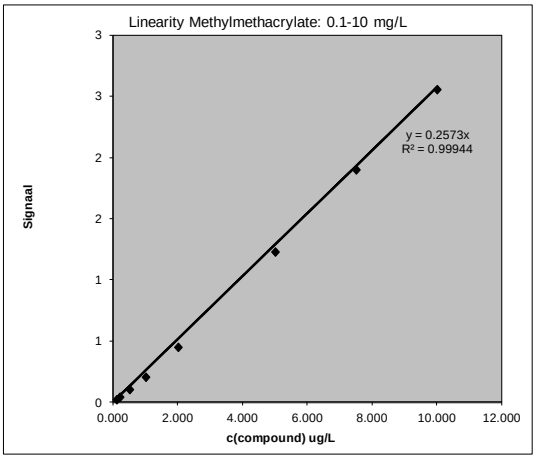

Linearity 1,1-Dichloropropene: 0.1-10 mg/L
y = 0.3303x
R² = 0.99971
Signaal
c(compound) ug/L

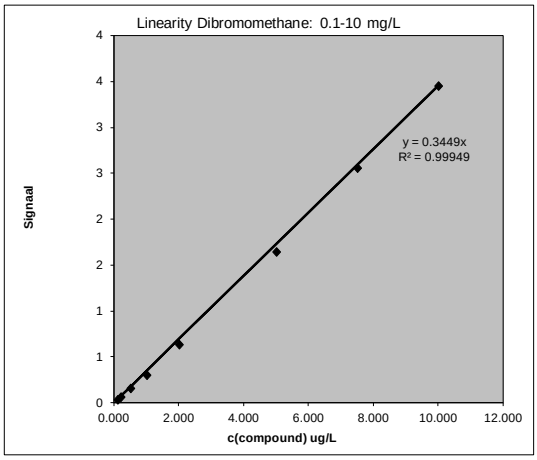
(Figure 2)

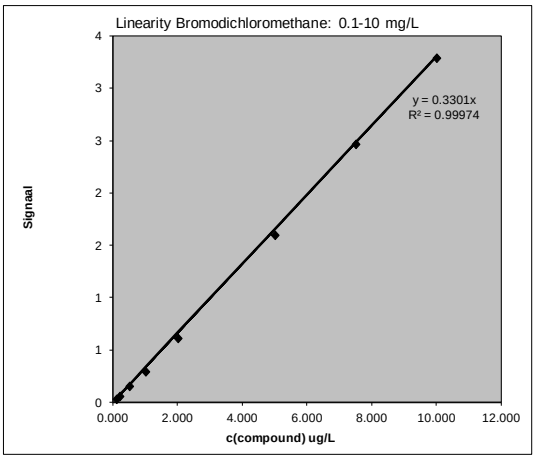

Linearity TAME: 0.1-10 mg/L
y = 0.6866x
R² = 0.99980
Signaal
c(compound) ug/L

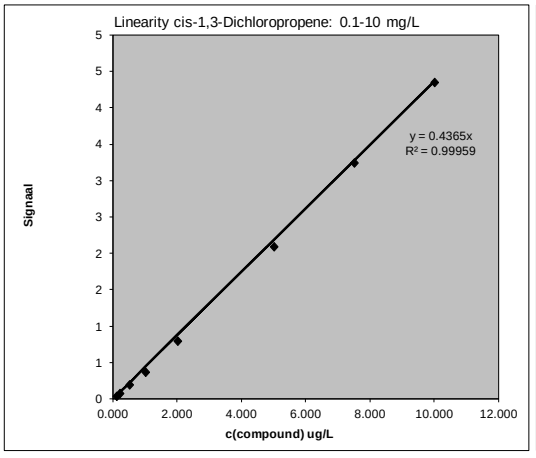

Linearity n-Heptane: 0.1-10 mg/L
y = 0.2828x
R² = 0.99929
Signaal
c(compound) ug/L

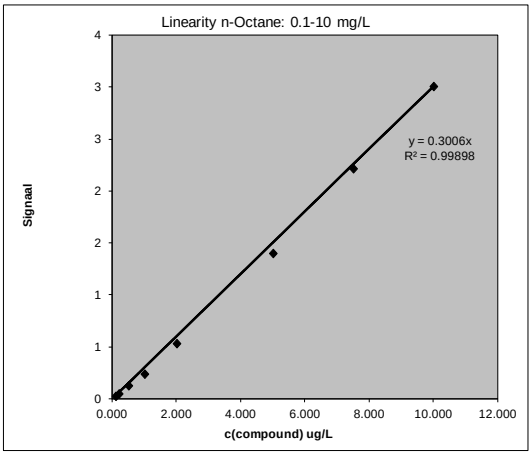

Linearity 2,3-dichloropropene: 0.1-10 mg/L
y = 0.4571x
R² = 0.99945
Signaal
c(compound) ug/L


Linearity Methylmethacrylate: 0.1-10 mg/L
y = 0.2573x
R² = 0.99944
Signaal
c(compound) ug/L

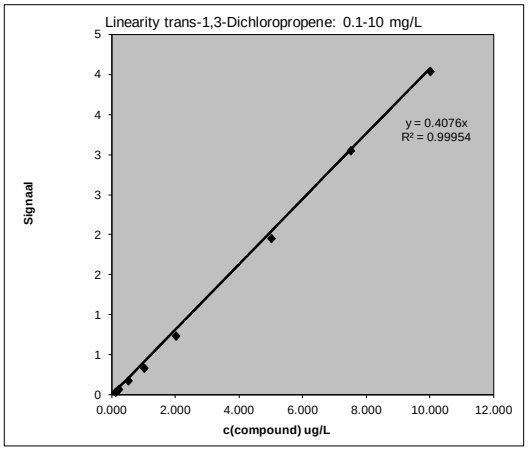

Linearity Dibromomethane: 0.1-10 mg/L
y = 0.3449x
R² = 0.99949
Signaal
c(compound) ug/L

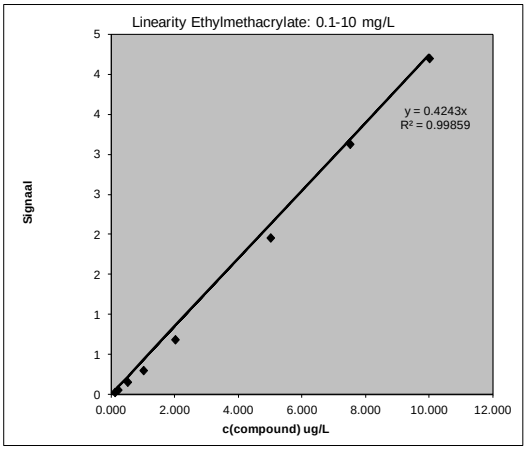

Linearity Bromodichloromethane: 0.1-10 mg/L
y = 0.3301x
R² = 0.99974
Signaal
c(compound) ug/L

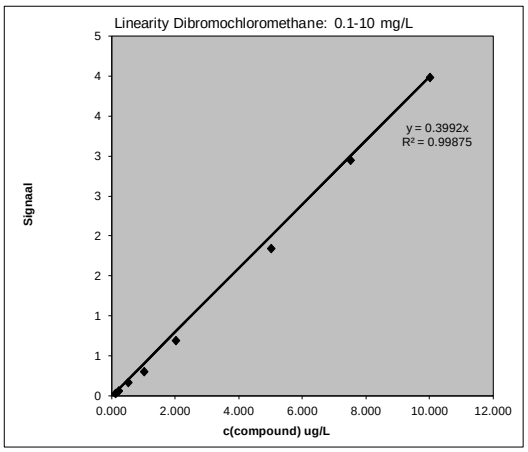

Linearity cis-1,3-Dichloropropene: 0.1-10 mg/L
y = 0.4365x
R² = 0.99959
Signaal
c(compound) ug/L

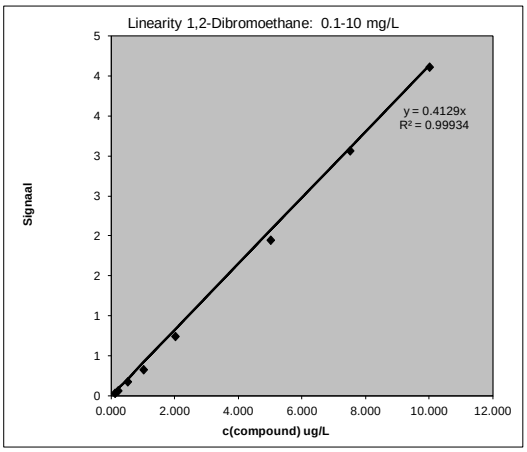

Linearity n-Octane: 0.1-10 mg/L
y = 0.3006x
R² = 0.99898
Signaal
c(compound) ug/L

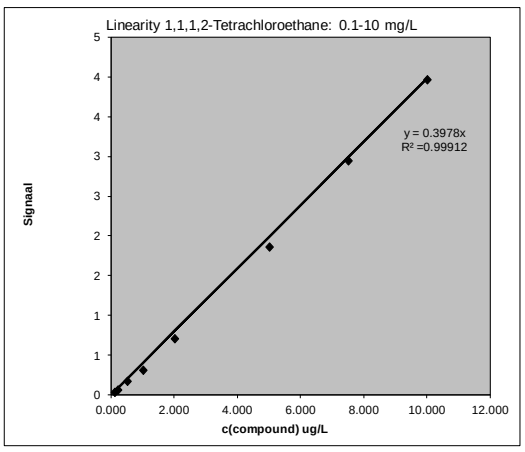
(Figure 2)

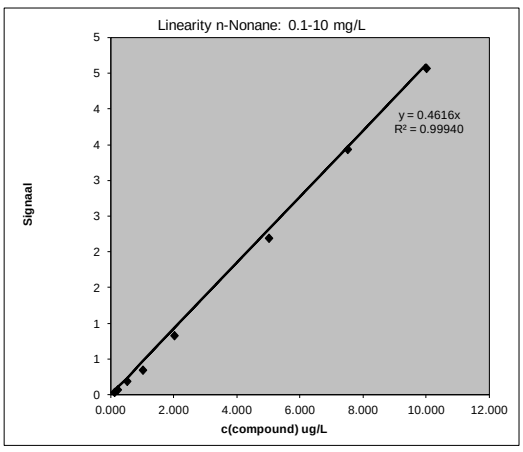

Linearity trans-1,3-Dichloropropene: 0.1-10 mg/L
y = 0.4076x
R² = 0.99954
Signaal
c(compound) ug/L


Linearity Ethylmethacrylate: 0.1-10 mg/L
y = 0.4243x
R² = 0.99859
Signaal
c(compound) ug/L

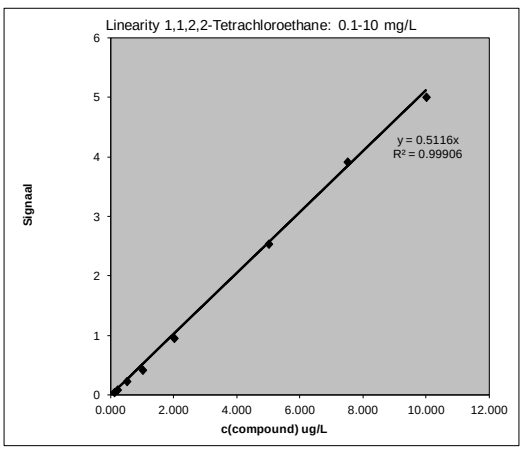

Linearity Dibromochloromethane: 0.1-10 mg/L
y = 0.3992x
R² = 0.99875
Signaal
c(compound) ug/L


Linearity 1,2-Dibromoethane: 0.1-10 mg/L
y = 0.4129x
R² = 0.99934
Signaal
c(compound) ug/L

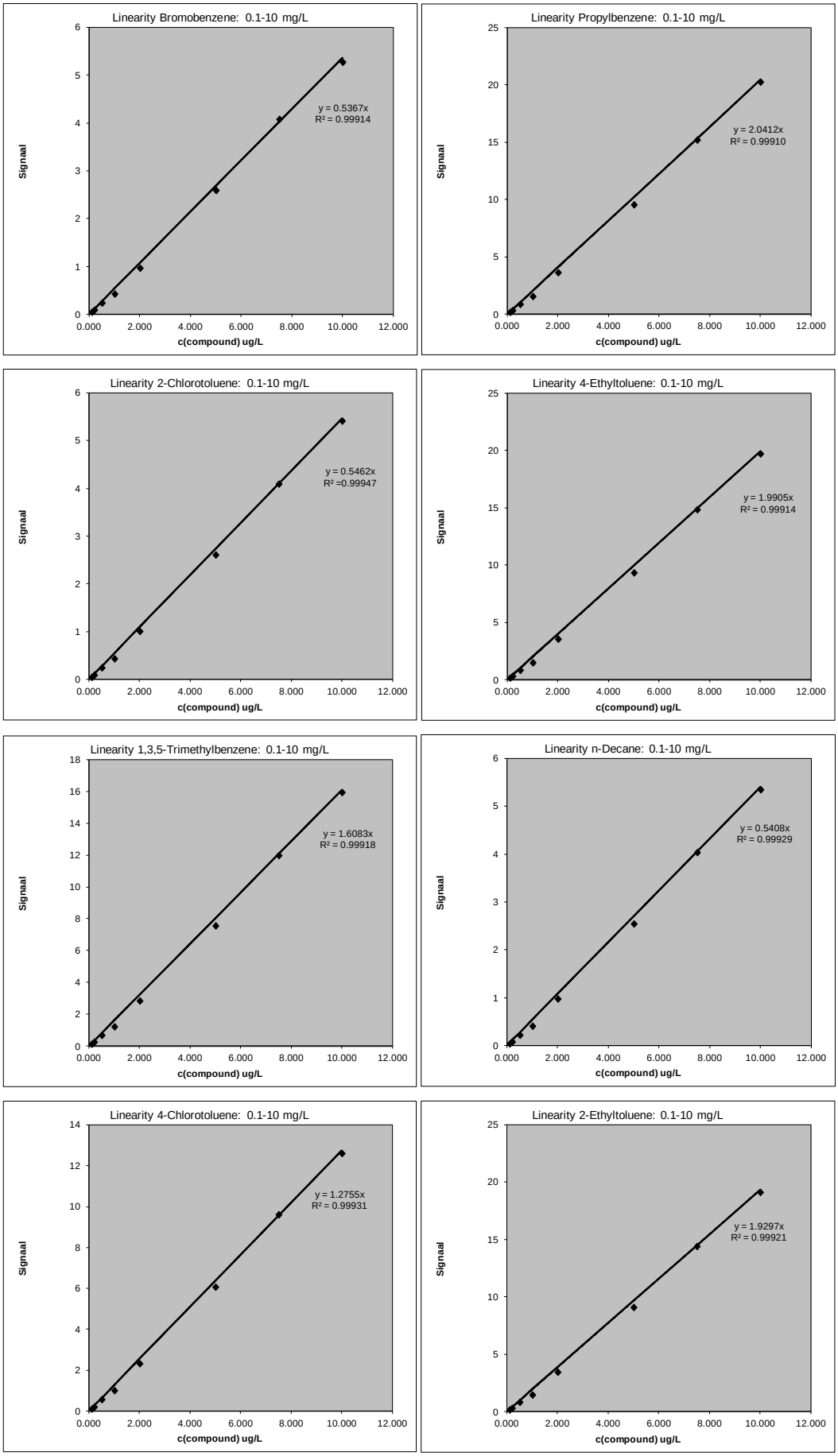

Linearity 1,1,1,2-Tetrachloroethane: 0.1-10 mg/L
y = 0.3978x
R² =0.99912
Signaal
c(compound) ug/L


Linearity n-Nonane: 0.1-10 mg/L
y = 0.4616x
R² = 0.99940
Signaal
c(compound) ug/L

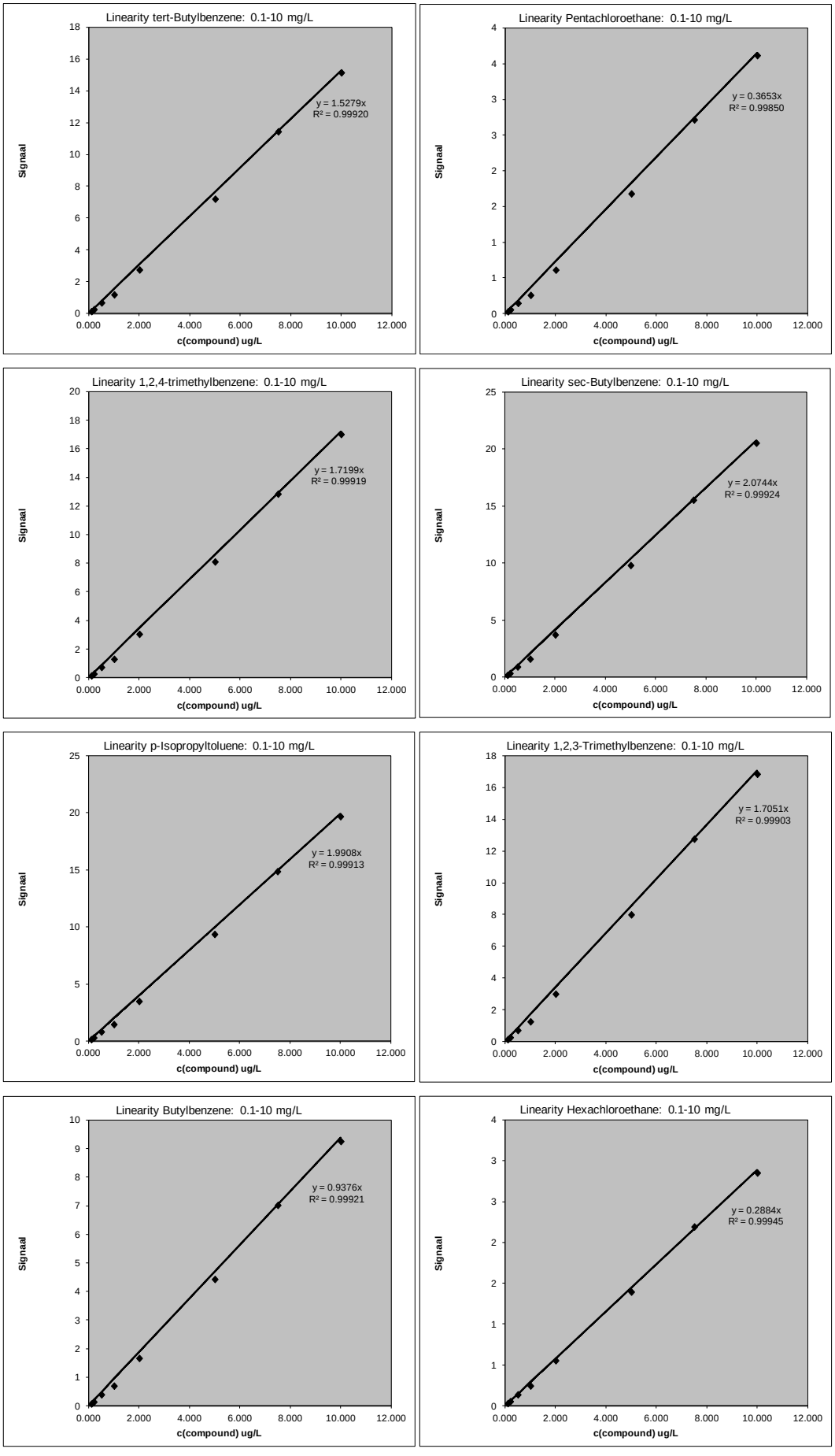

Linearity 3-Ethyltoluene: 0.1-10 mg/L
y = 2.0112x
R² = 0.99921
Signaal
c(compound) ug/L


Linearity 1,1,2,2-Tetrachloroethane: 0.1-10 mg/L
y = 0.5116x
R² = 0.99906
Signaal
c(compound) ug/L

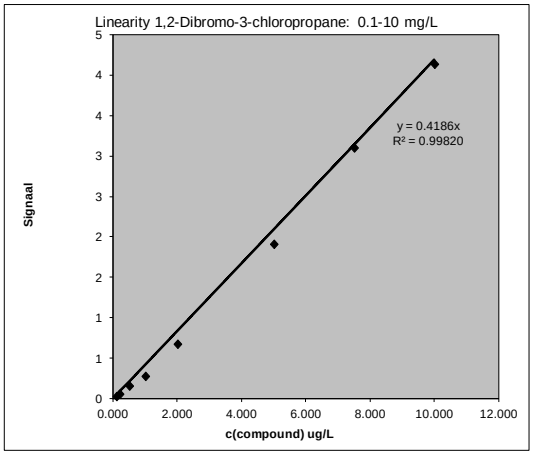
(Figure 2)

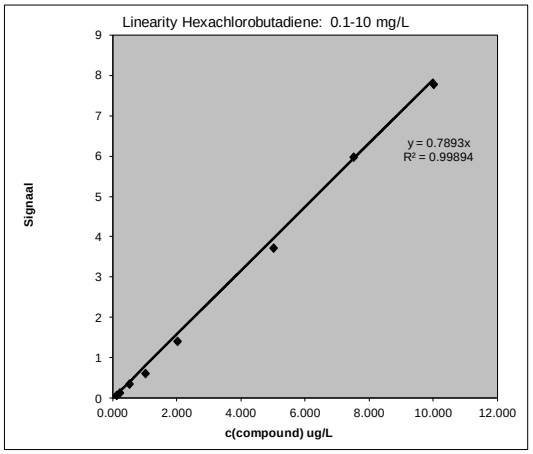

Linearity Bromobenzene: 0.1-10 mg/L
y = 0.5367x
R² = 0.99914
Linearity Propylbenzene: 0.1-10 mg/L
y = 2.0412x
R² = 0.99910
Linearity 2-Chlorotoluene: 0.1-10 mg/L
y = 0.5462x
R² =0.99947
Linearity 4-Ethyltoluene: 0.1-10 mg/L
y = 1.9905x
R² = 0.99914
Linearity 1,3,5-Trimethylbenzene: 0.1-10 mg/L
y = 1.6083x
R² = 0.99918
Linearity n-Decane: 0.1-10 mg/L
y = 0.5408x
R² = 0.99929
Linearity 4-Chlorotoluene: 0.1-10 mg/L
y = 1.2755x
R² = 0.99931
Linearity 2-Ethyltoluene: 0.1-10 mg/L
y = 1.9297x
R² = 0.99921
Signaal
c(compound) ug/L

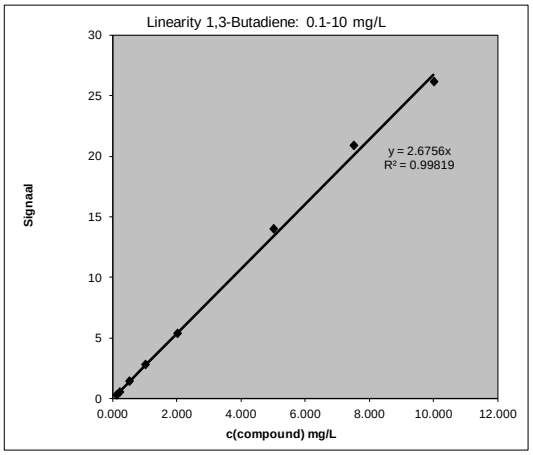
(Figure 2)

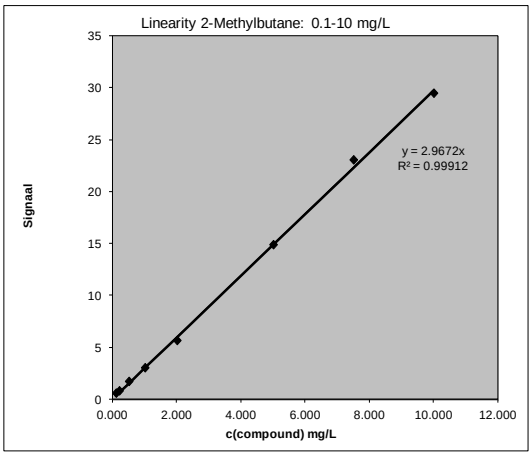

Linearity tert-Butylbenzene: 0.1-10 mg/L
y = 1.5279x
R² = 0.99920
Linearity Pentachloroethane: 0.1-10 mg/L
y = 0.3653x
R² = 0.99850
Linearity 1,2,4-trimethylbenzene: 0.1-10 mg/L
y = 1.7199x
R² = 0.99919
Linearity sec-Butylbenzene: 0.1-10 mg/L
y = 2.0744x
R² = 0.99924
Linearity p-Isopropyltoluene: 0.1-10 mg/L
y = 1.9908x
R² = 0.99913
Linearity 1,2,3-Trimethylbenzene: 0.1-10 mg/L
y = 1.7051x
R² = 0.99903
Linearity Butylbenzene: 0.1-10 mg/L
y = 0.9376x
R² = 0.99921
Linearity Hexachloroethane: 0.1-10 mg/L
y = 0.2884x
R² = 0.99945
Signaal
c(compound) ug/L

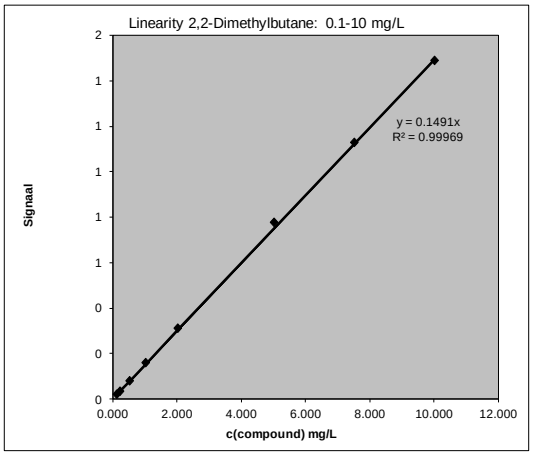
(Figure 2)

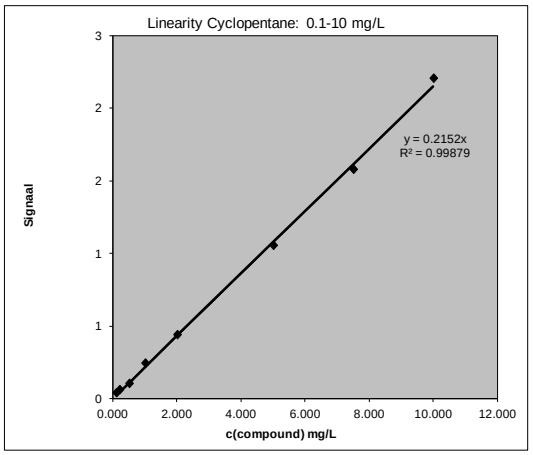

Linearity 1,2-Dibromo-3-chloropropane: 0.1-10 mg/L
y = 0.4186x
R² = 0.99820
Signaal
c(compound) ug/L

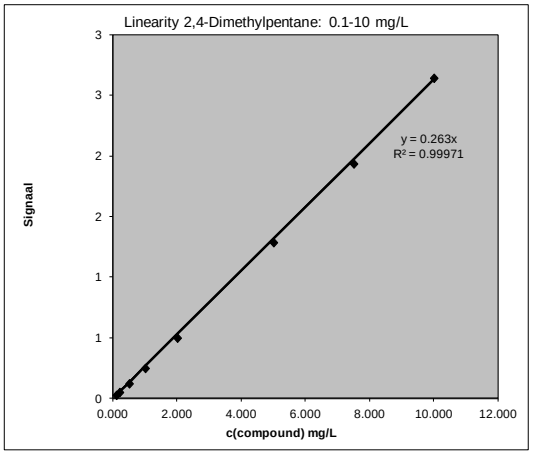

Linearity Hexachlorobutadiene: 0.1-10 mg/L
y = 0.7893x
R² = 0.99894
Signaal
c(compound) ug/L

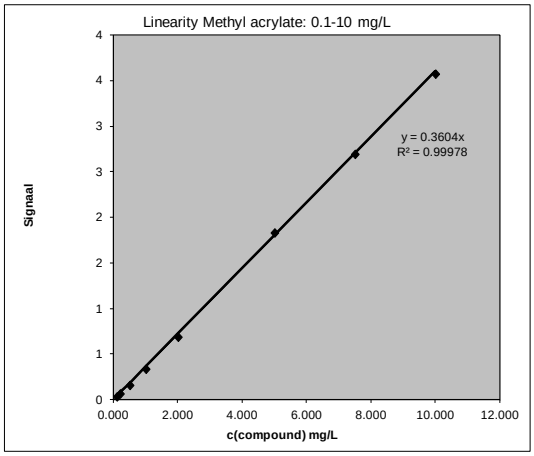

Linearity 1,3-Butadiene: 0.1-10 mg/L
y = 2.6756x
R² = 0.99819
Signaal
c(compound) mg/L


Linearity 2-Methylbutane: 0.1-10 mg/L
y = 2.9672x
R² = 0.99912
Signaal
c(compound) mg/L

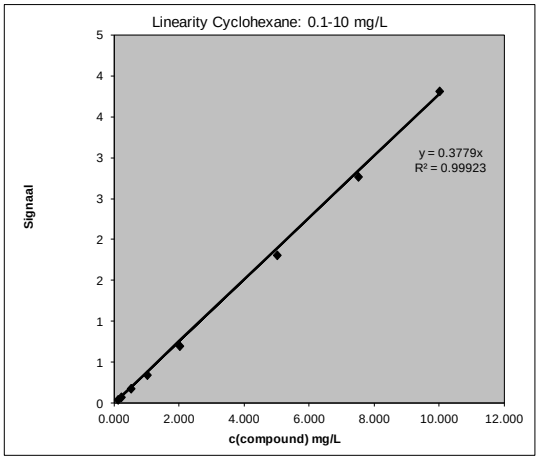

Linearity 2,2-Dimethylbutane: 0.1-10 mg/L
y = 0.1491x
R² = 0.99969
Signaal
c(compound) mg/L

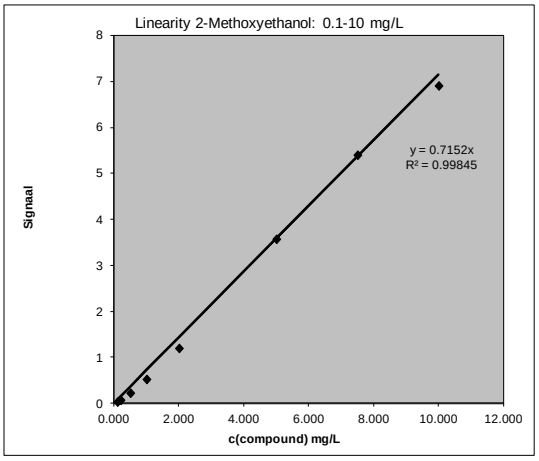

Linearity Cyclopentane: 0.1-10 mg/L
y = 0.2152x
R² = 0.99879
Signaal
c(compound) mg/L

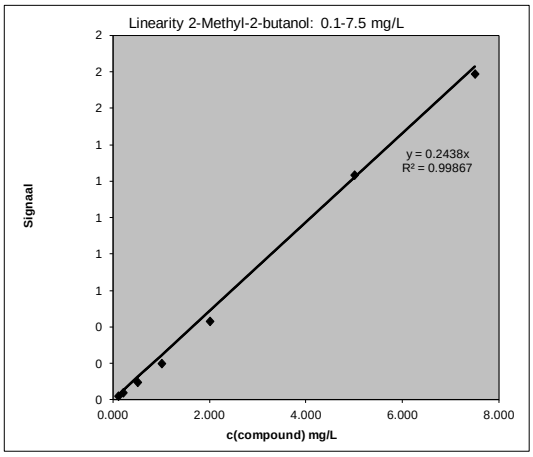

Linearity 2,4-Dimethylpentane: 0.1-10 mg/L
y = 0.263x
R² = 0.99971
Signaal
c(compound) mg/L

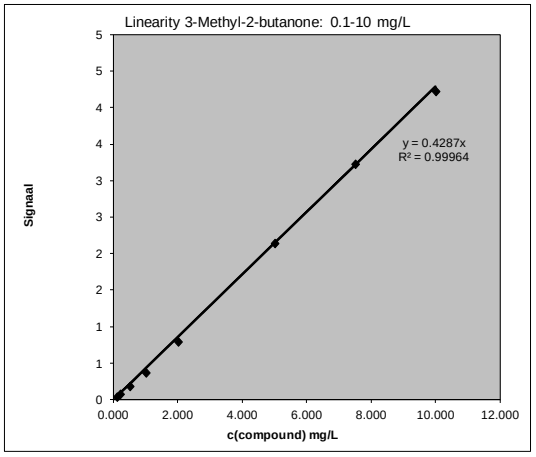

Linearity Methyl acrylate: 0.1-10 mg/L
y = 0.3604x
R² = 0.99978
Signaal
c(compound) mg/L

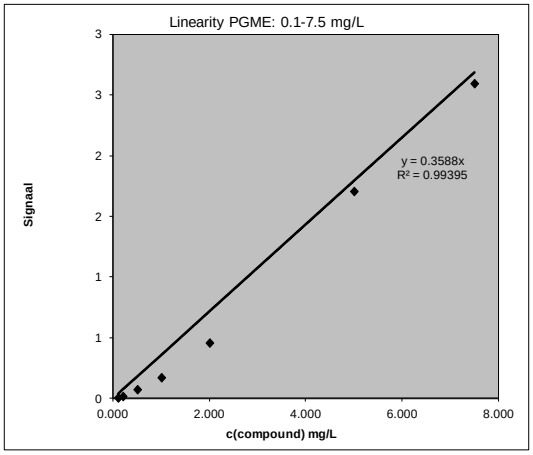
(Figure 2)

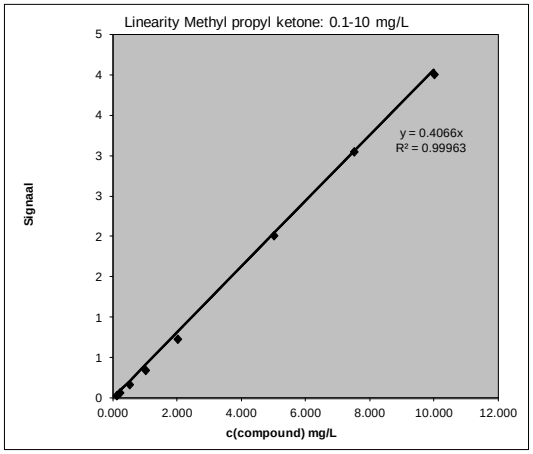

Linearity Cyclohexane: 0.1-10 mg/L
y = 0.3779x
R² = 0.99923
Signaal
c(compound) mg/L

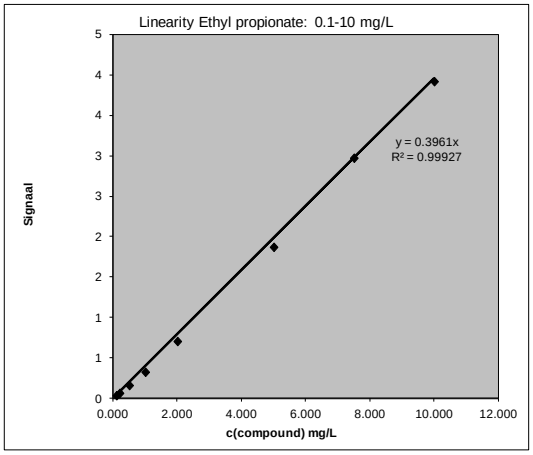

Linearity 2-Methoxyethanol: 0.1-10 mg/L
y = 0.7152x
R² = 0.99845
Signaal
c(compound) mg/L

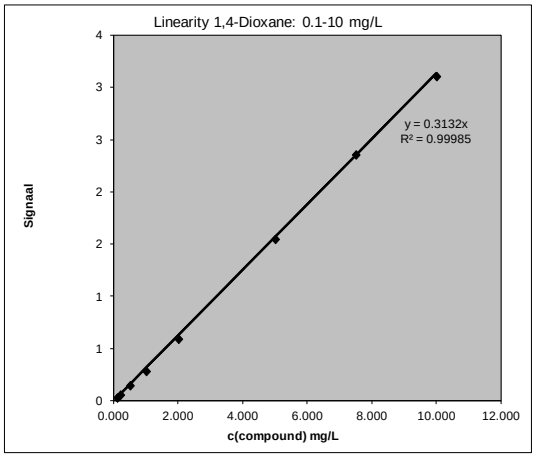

Linearity 2-Methyl-2-butanol: 0.1-7.5 mg/L
y = 0.2438x
R² = 0.99867
Signaal
c(compound) mg/L


Linearity 3-Methyl-2-butanone: 0.1-10 mg/L
y = 0.4287x
R² = 0.99964
Signaal
c(compound) mg/L

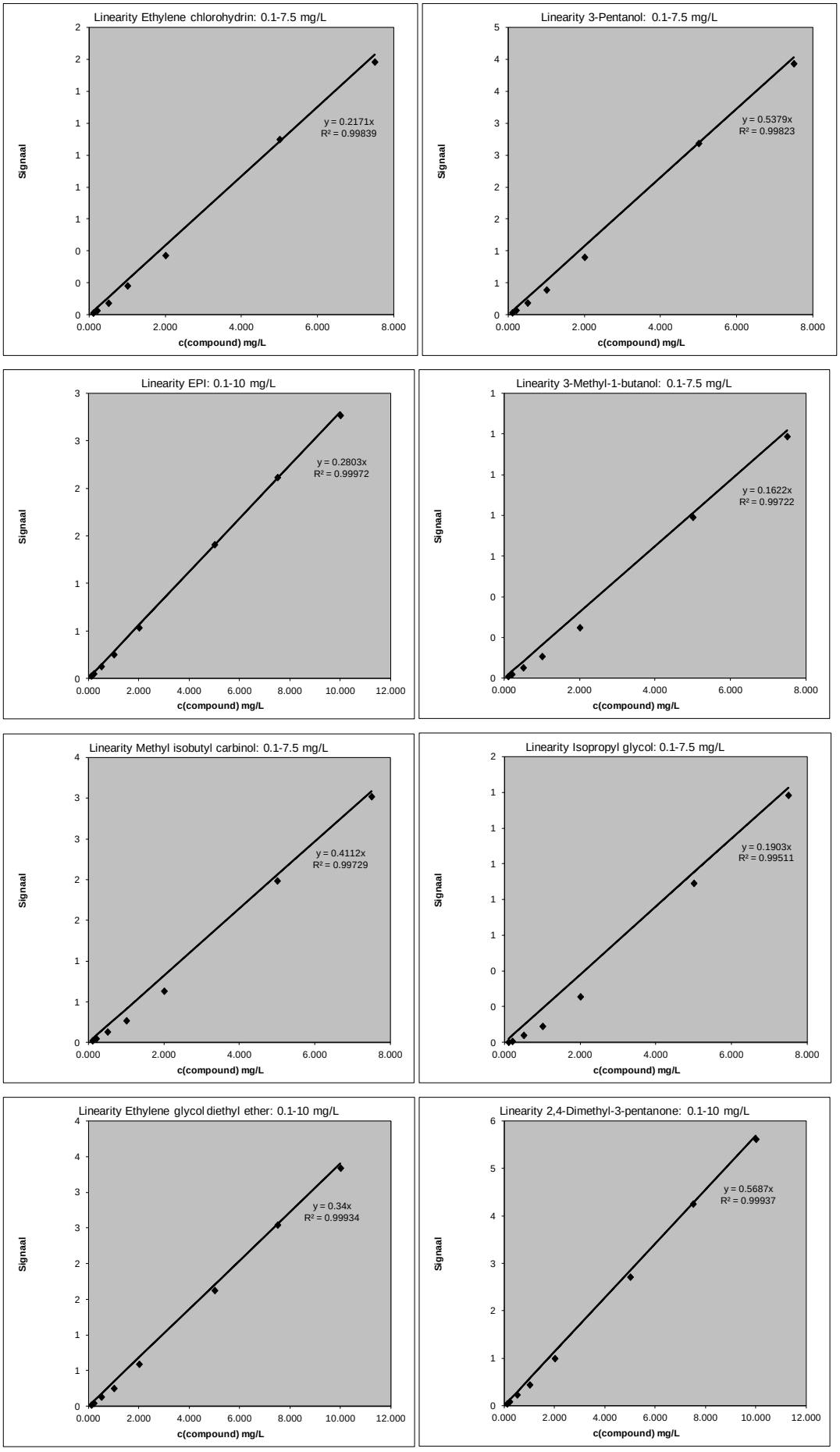

Linearity PGME: 0.1-7.5 mg/L
y = 0.3588x
R² = 0.99395
Signaal
c(compound) mg/L


Linearity Methyl propyl ketone: 0.1-10 mg/L
y = 0.4066x
R² = 0.99963
Signaal
c(compound) mg/L

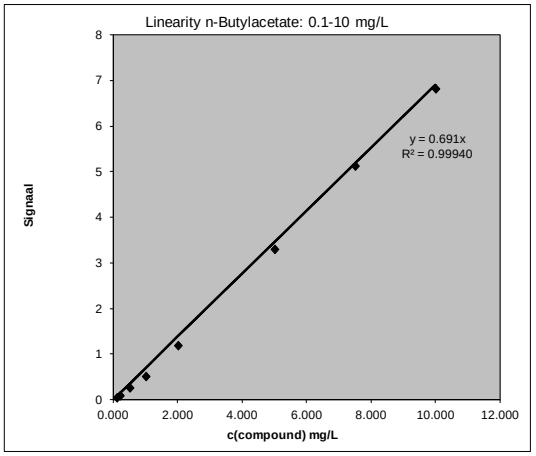

Linearity Ethyl propionate: 0.1-10 mg/L
y = 0.3961x
R² = 0.99927
Signaal
c(compound) mg/L

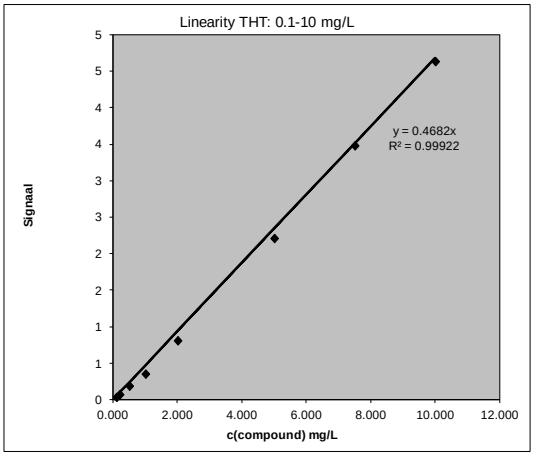

Linearity 1,4-Dioxane: 0.1-10 mg/L
y = 0.3132x
R² = 0.99985
Signaal
c(compound) mg/L

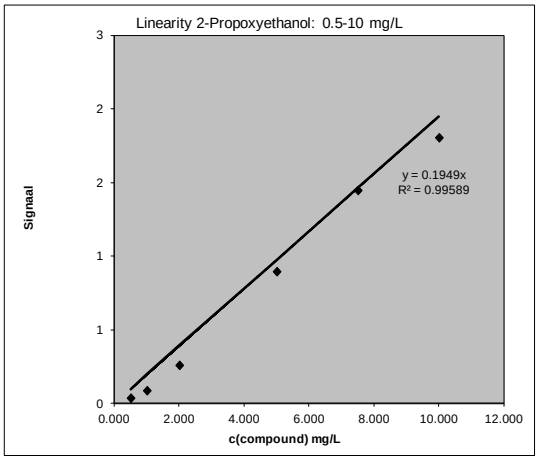
(Figure 2)

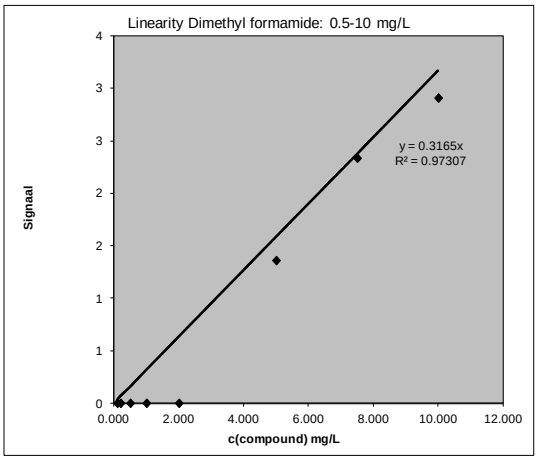

Linearity Ethylene chlorohydrin: 0.1-7.5 mg/L
y = 0.2171x
R² = 0.99839
Signaal
c(compound) mg/L
Linearity 3-Pentanol: 0.1-7.5 mg/L
y = 0.5379x
R² = 0.99823
Signaal
c(compound) mg/L
Linearity EPI: 0.1-10 mg/L
y = 0.2803x
R² = 0.99972
Signaal
c(compound) mg/L
Linearity 3-Methyl-1-butanol: 0.1-7.5 mg/L
y = 0.1622x
R² = 0.99722
Signaal
c(compound) mg/L
Linearity Methyl isobutyl carbinol: 0.1-7.5 mg/L
y = 0.4112x
R² = 0.99729
Signaal
c(compound) mg/L
Linearity Isopropyl glycol: 0.1-7.5 mg/L
y = 0.1903x
R² = 0.99511
Signaal
c(compound) mg/L
Linearity Ethylene glycol diethyl ether: 0.1-10 mg/L
y = 0.34x
R² = 0.99934
Signaal
c(compound) mg/L
Linearity 2,4-Dimethyl-3-pentanone: 0.1-10 mg/L
y = 0.5687x
R² = 0.99937
Signaal
c(compound) mg/L

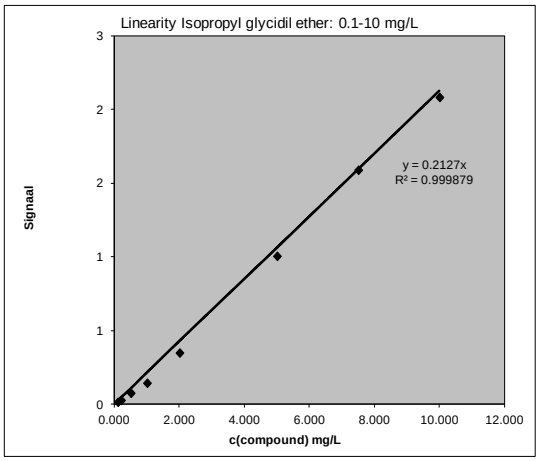
(Figure 2)

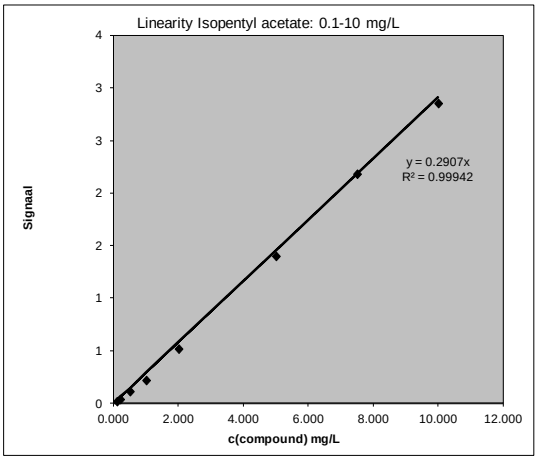

Linearity n-Butylacetate: 0.1-10 mg/L
y = 0.691x
R² = 0.99940
Signaal
c(compound) mg/L

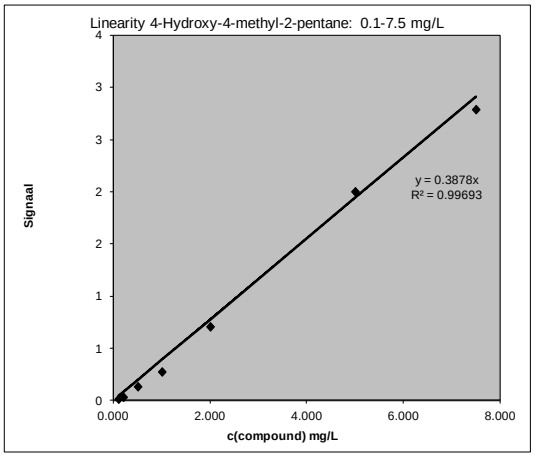

Linearity THT: 0.1-10 mg/L
y = 0.4682x
R² = 0.99922
Signaal
c(compound) mg/L

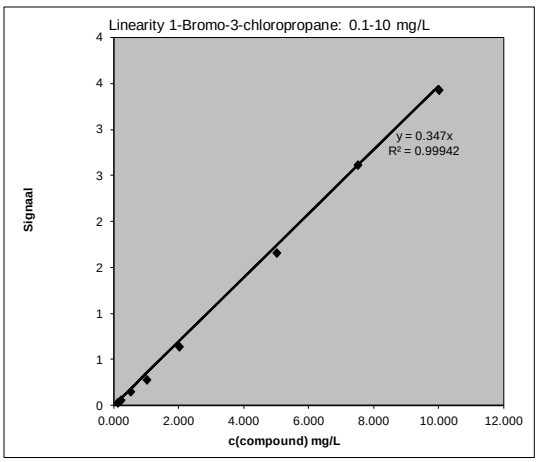

Linearity 2-Propoxyethanol: 0.5-10 mg/L
y = 0.1949x
R² = 0.99589
Signaal
c(compound) mg/L


Linearity Dimethyl formamide: 0.5-10 mg/L
y = 0.3165x
R² = 0.97307
Signaal
c(compound) mg/L

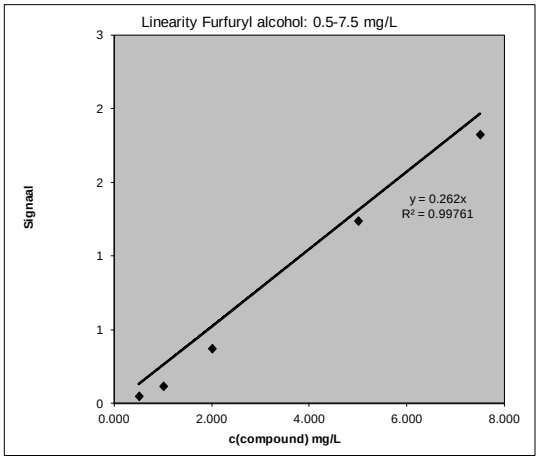

Linearity Isopropyl glycidil ether: 0.1-10 mg/L
y = 0.2127x
R² = 0.999879
Signaal
c(compound) mg/L

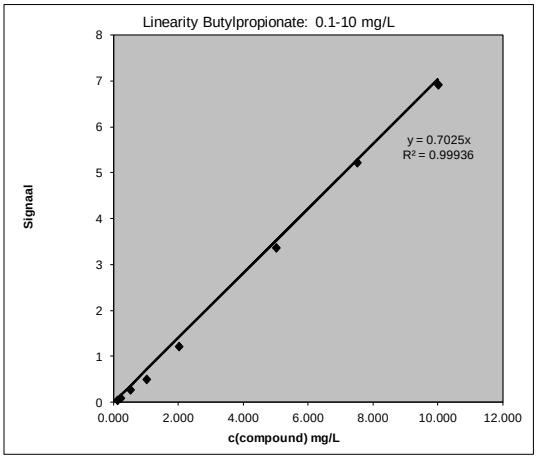

Linearity Isopentyl acetate: 0.1-10 mg/L
y = 0.2907x
R² = 0.99942
Signaal
c(compound) mg/L

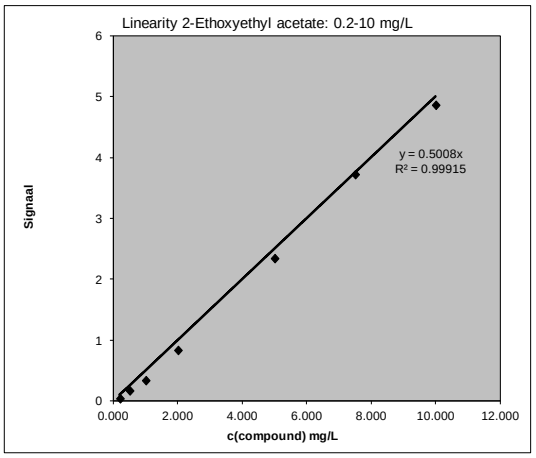

Linearity 4-Hydroxy-4-methyl-2-pentane: 0.1-7.5 mg/L
y = 0.3878x
R² = 0.99693
Signaal
c(compound) mg/L

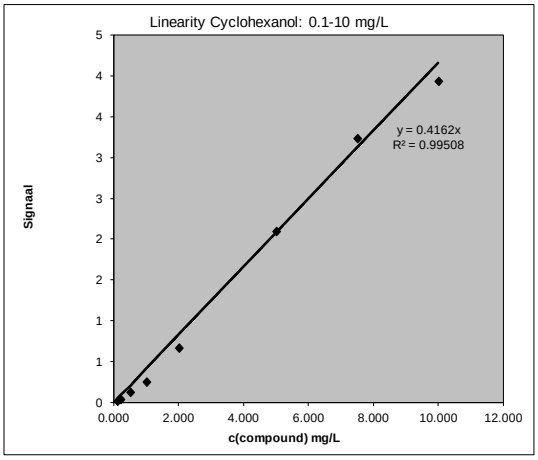

Linearity 1-Bromo-3-chloropropane: 0.1-10 mg/L
y = 0.347x
R² = 0.99942
Signaal
c(compound) mg/L

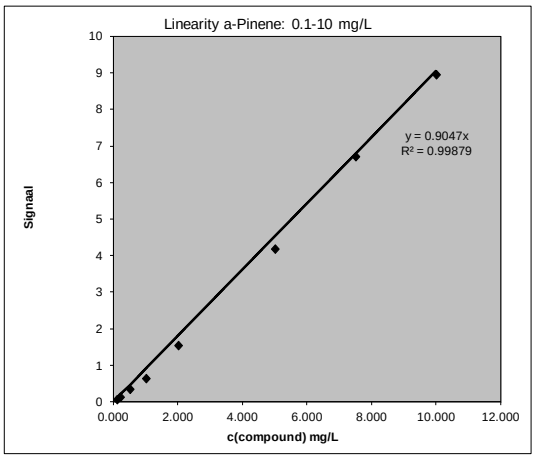
(Figure 2)

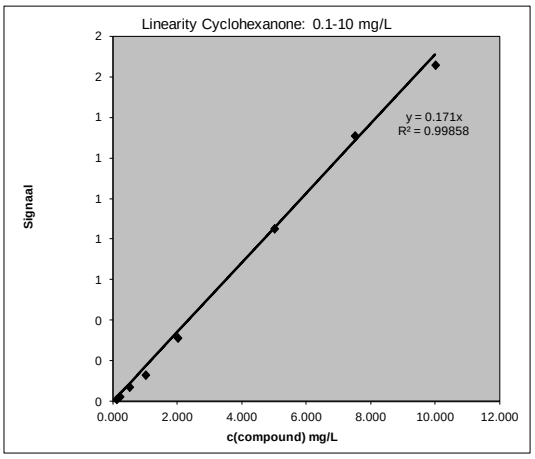

Linearity Furfuryl alcohol: 0.5-7.5 mg/L
Signaal
c(compound) mg/L
y = 0.262x
R² = 0.99761

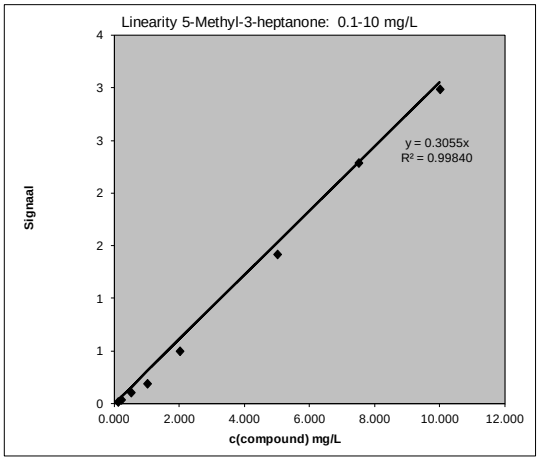

Linearity Butylpropionate: 0.1-10 mg/L
Signaal
c(compound) mg/L
y = 0.7025x
R² = 0.99936

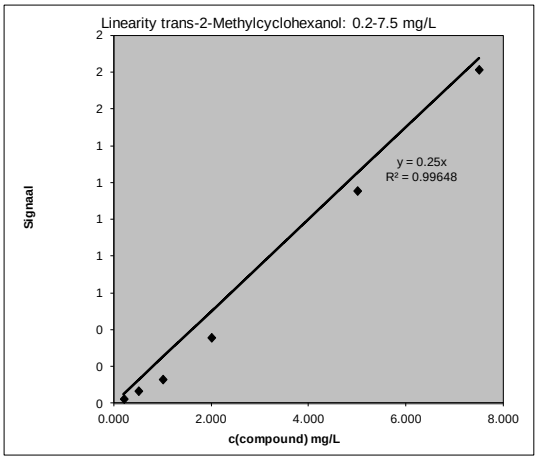

Linearity 2-Ethoxyethyl acetate: 0.2-10 mg/L
Signaal
c(compound) mg/L
y = 0.5008x
R² = 0.99915


Linearity Cyclohexanol: 0.1-10 mg/L
Signaal
c(compound) mg/L
y = 0.4162x
R² = 0.99508

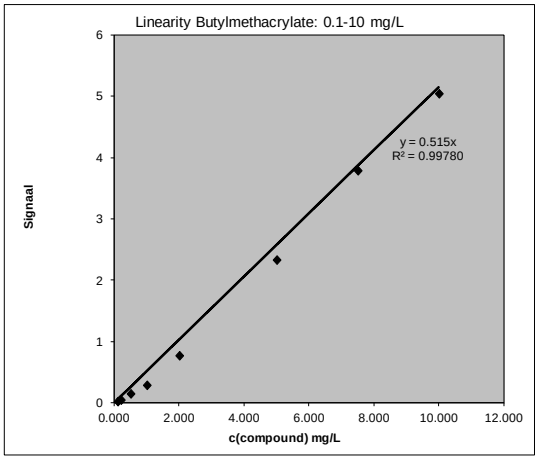

Linearity a-Pinene: 0.1-10 mg/L
Signaal
c(compound) mg/L
y = 0.9047x
R² = 0.99879

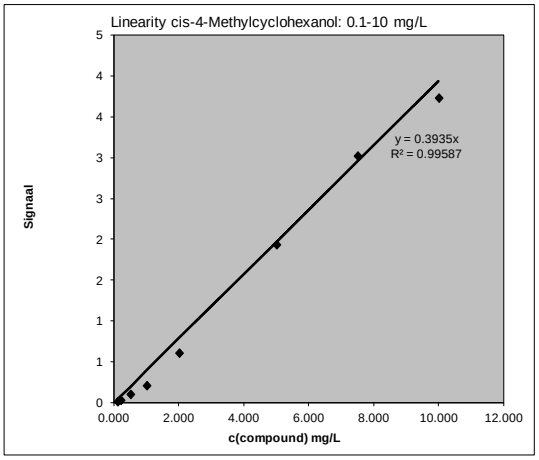

Linearity Cyclohexanone: 0.1-10 mg/L
Signaal
c(compound) mg/L
y = 0.171x
R² = 0.99858

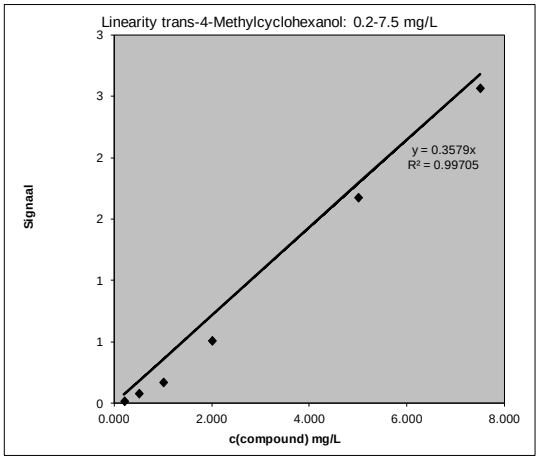

Linearity 5-Methyl-3-heptanone: 0.1-10 mg/L
Signaal
c(compound) mg/L
y = 0.3055x
R² = 0.99840

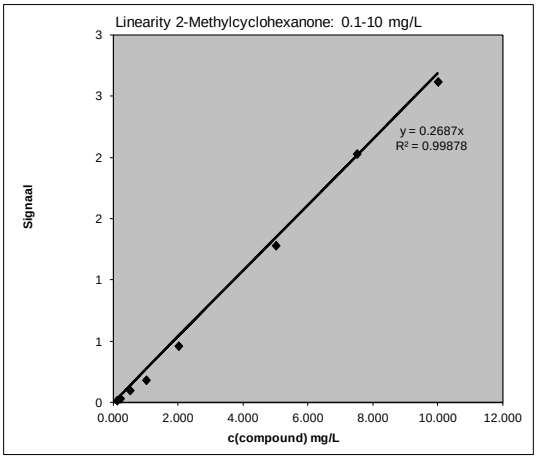

Linearity trans-2-Methylcyclohexanol: 0.2-7.5 mg/L
Signaal
c(compound) mg/L
y = 0.25x
R² = 0.99648

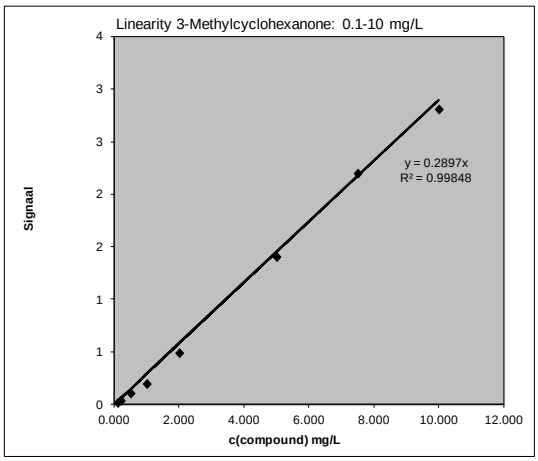
(Figure 2)

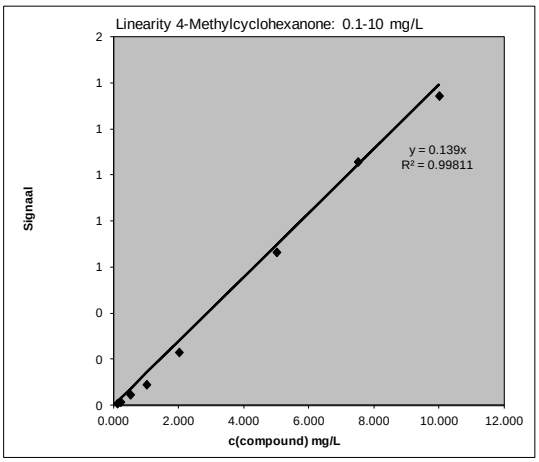

Linearity Butylmethacrylate: 0.1-10 mg/L
y = 0.515x
R² = 0.99780
Signaal
c(compound) mg/L

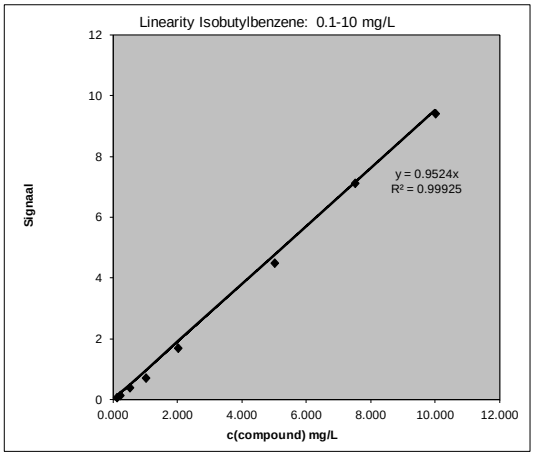

Linearity cis-4-Methylcyclohexanol: 0.1-10 mg/L
y = 0.3935x
R² = 0.99587
Signaal
c(compound) mg/L

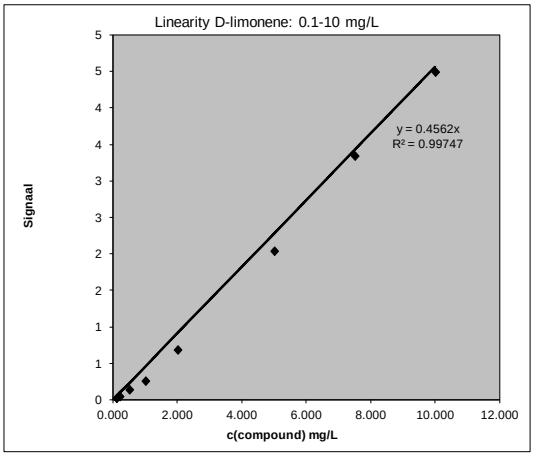

Linearity trans-4-Methylcyclohexanol: 0.2-7.5 mg/L
y = 0.3579x
R² = 0.99705
Signaal
c(compound) mg/L


Linearity 2-Methylcyclohexanone: 0.1-10 mg/L
y = 0.2687x
R² = 0.99878
Signaal
c(compound) mg/L

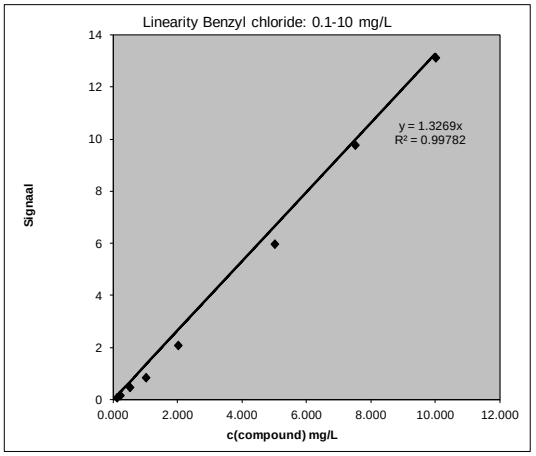

Linearity 3-Methylcyclohexanone: 0.1-10 mg/L
y = 0.2897x
R² = 0.99848
Signaal
c(compound) mg/L

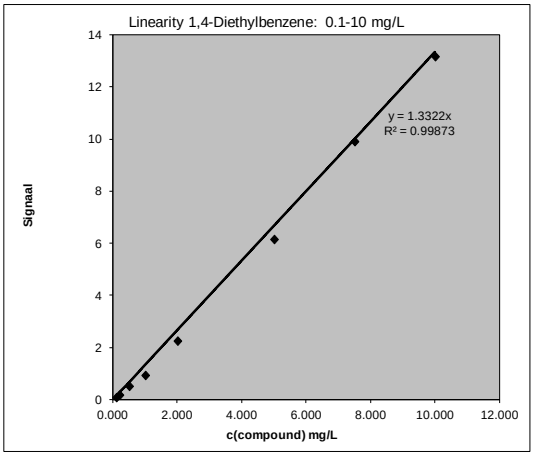

Linearity 4-Methylcyclohexanone: 0.1-10 mg/L
y = 0.139x
R² = 0.99811
Signaal
c(compound) mg/L

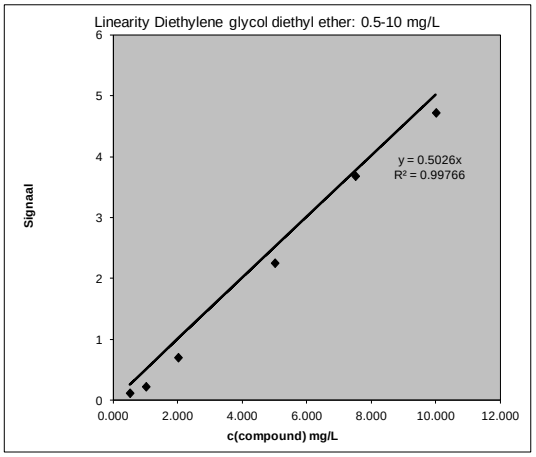

Linearity Isobutylbenzene: 0.1-10 mg/L
y = 0.9524x
R² = 0.99925
Signaal
c(compound) mg/L

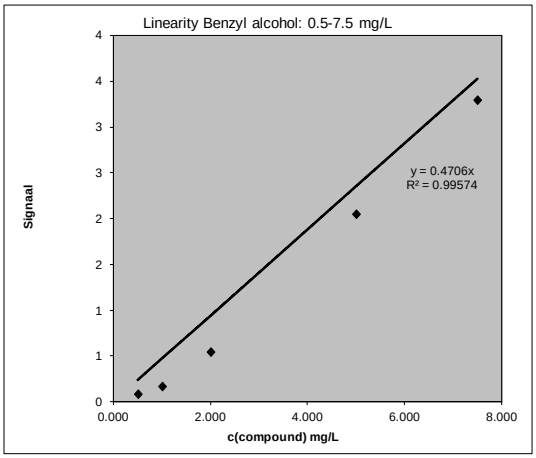

Linearity D-limonene: 0.1-10 mg/L
y = 0.4562x
R² = 0.99747
Signaal
c(compound) mg/L

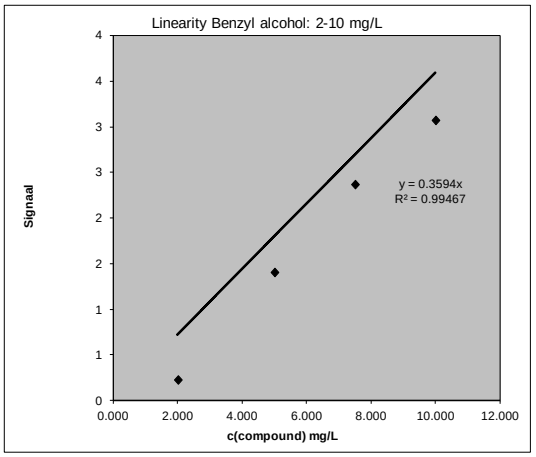
(Figure 2)

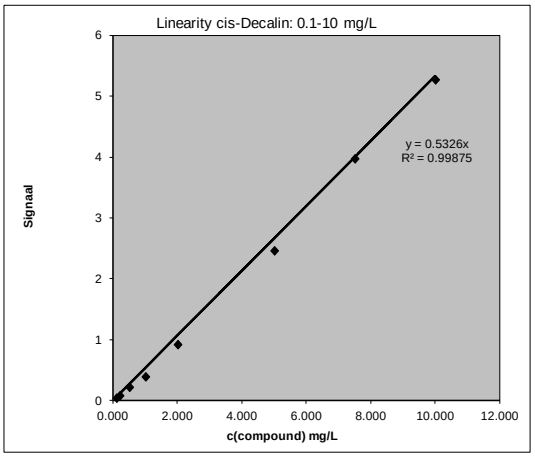

Linearity Benzyl chloride: 0.1-10 mg/L
y = 1.3269x
R² = 0.99782
Signaal
c(compound) mg/L

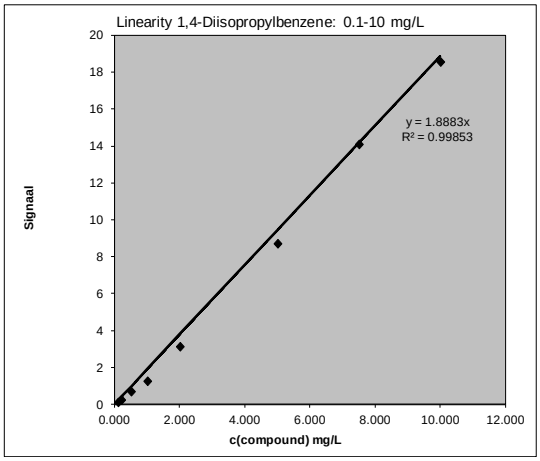

Linearity 1,4-Diethylbenzene: 0.1-10 mg/L
y = 1.3322x
R² = 0.99873
Signaal
c(compound) mg/L

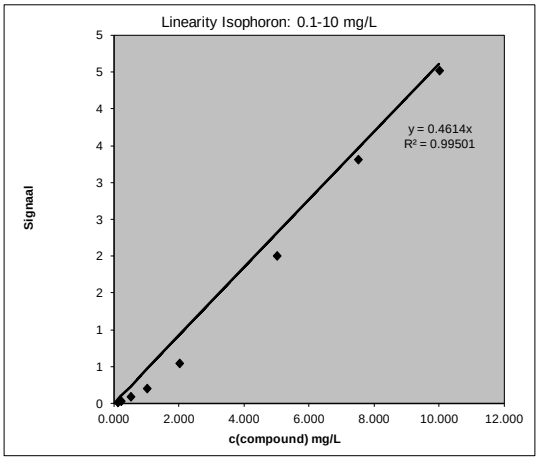

Linearity Diethylene glycol diethyl ether: 0.5-10 mg/L
y = 0.5026x
R² = 0.99766
Signaal
c(compound) mg/L


Linearity Benzyl alcohol: 0.5-7.5 mg/L
y = 0.4706x
R² = 0.99574
Signaal
c(compound) mg/L

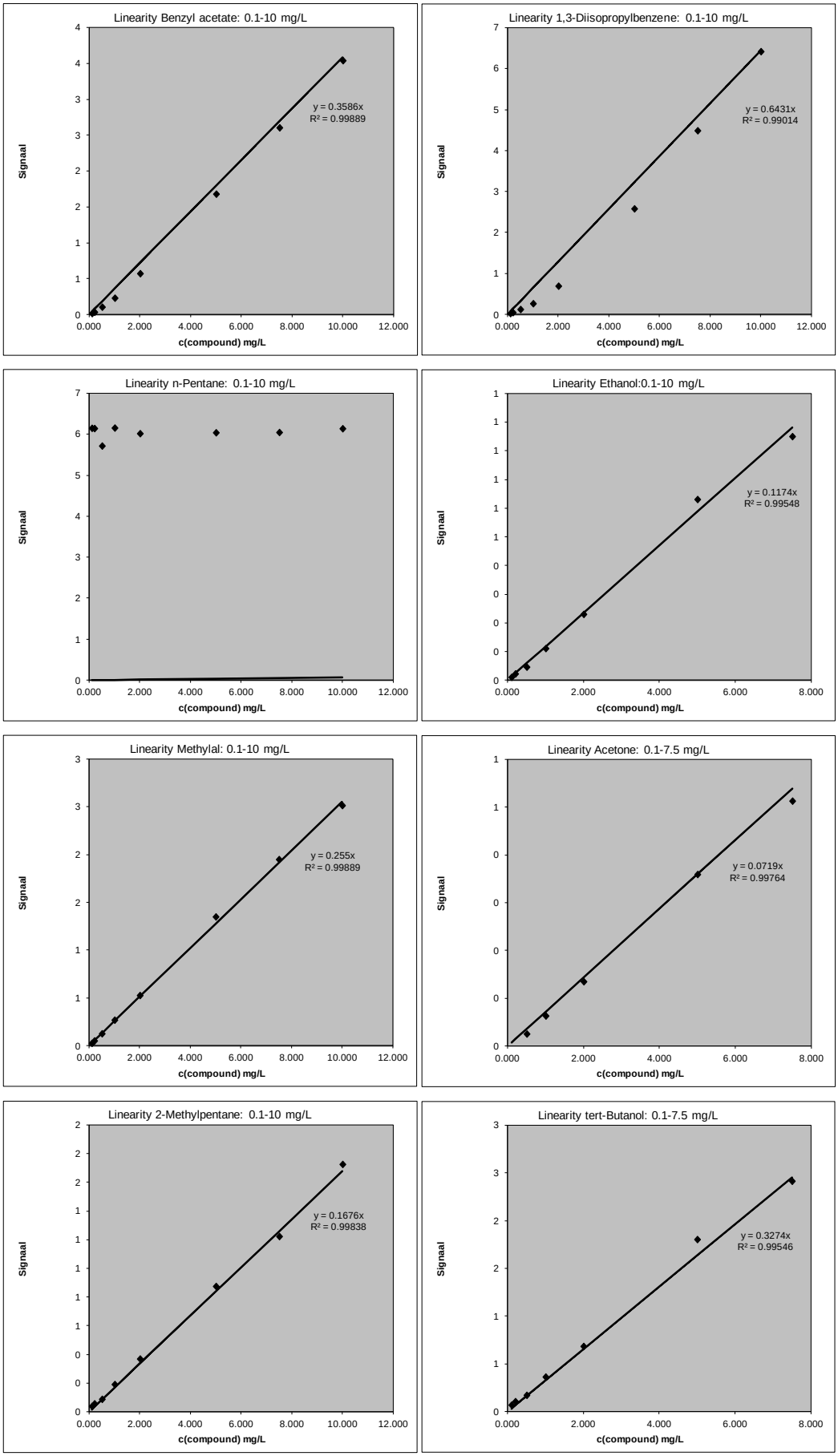

Linearity Benzyl alcohol: 2-10 mg/L
y = 0.3594x
R² = 0.99467
Signaal
c(compound) mg/L


Linearity cis-Decalin: 0.1-10 mg/L
y = 0.5326x
R² = 0.99875
Signaal
c(compound) mg/L

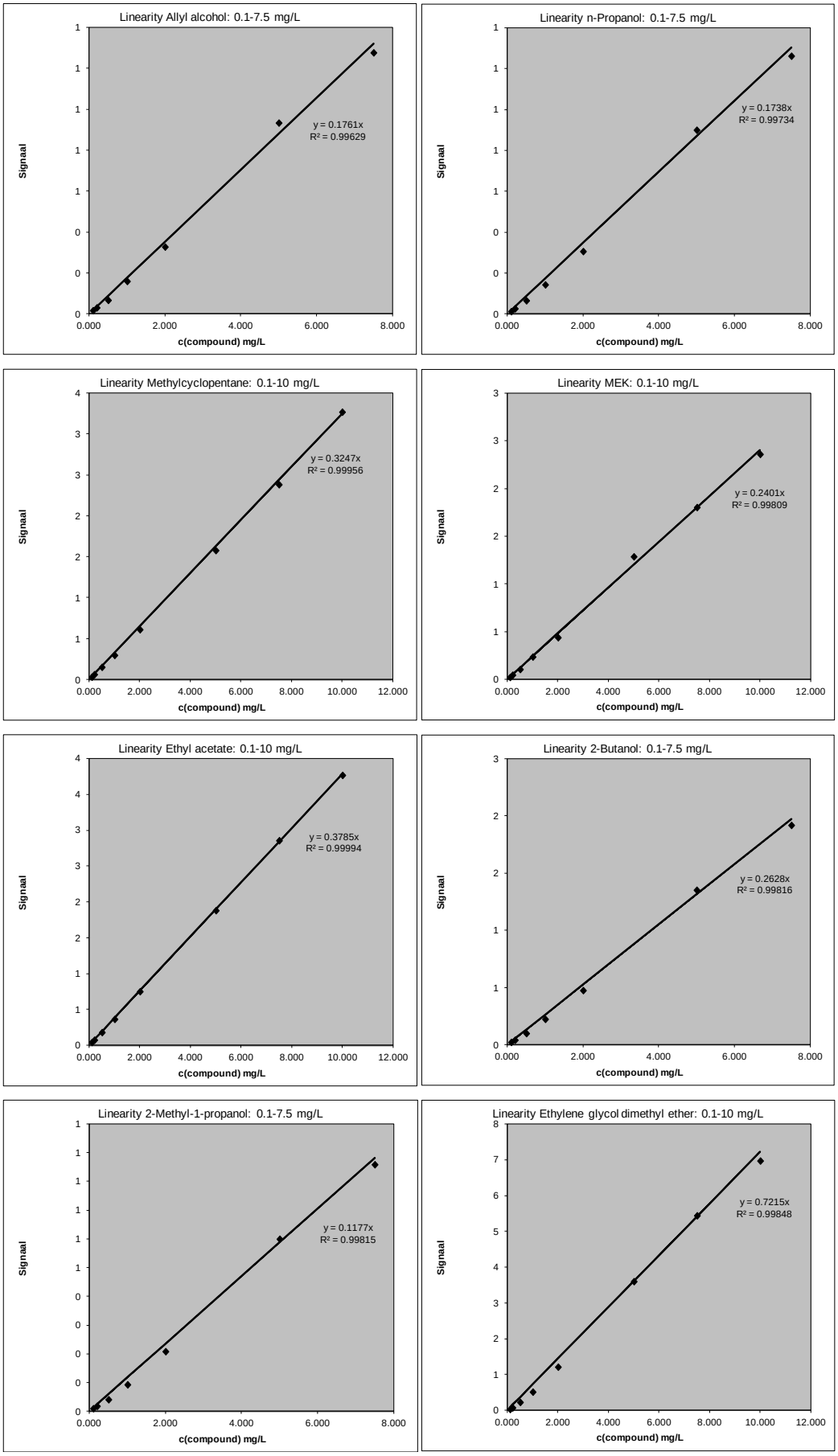

Linearity 1,4-Diisopropylbenzene: 0.1-10 mg/L
y = 1.8883x
R² = 0.99853
Signaal
c(compound) mg/L


Linearity Isophoron: 0.1-10 mg/L
y = 0.4614x
R² = 0.99501
Signaal
c(compound) mg/L

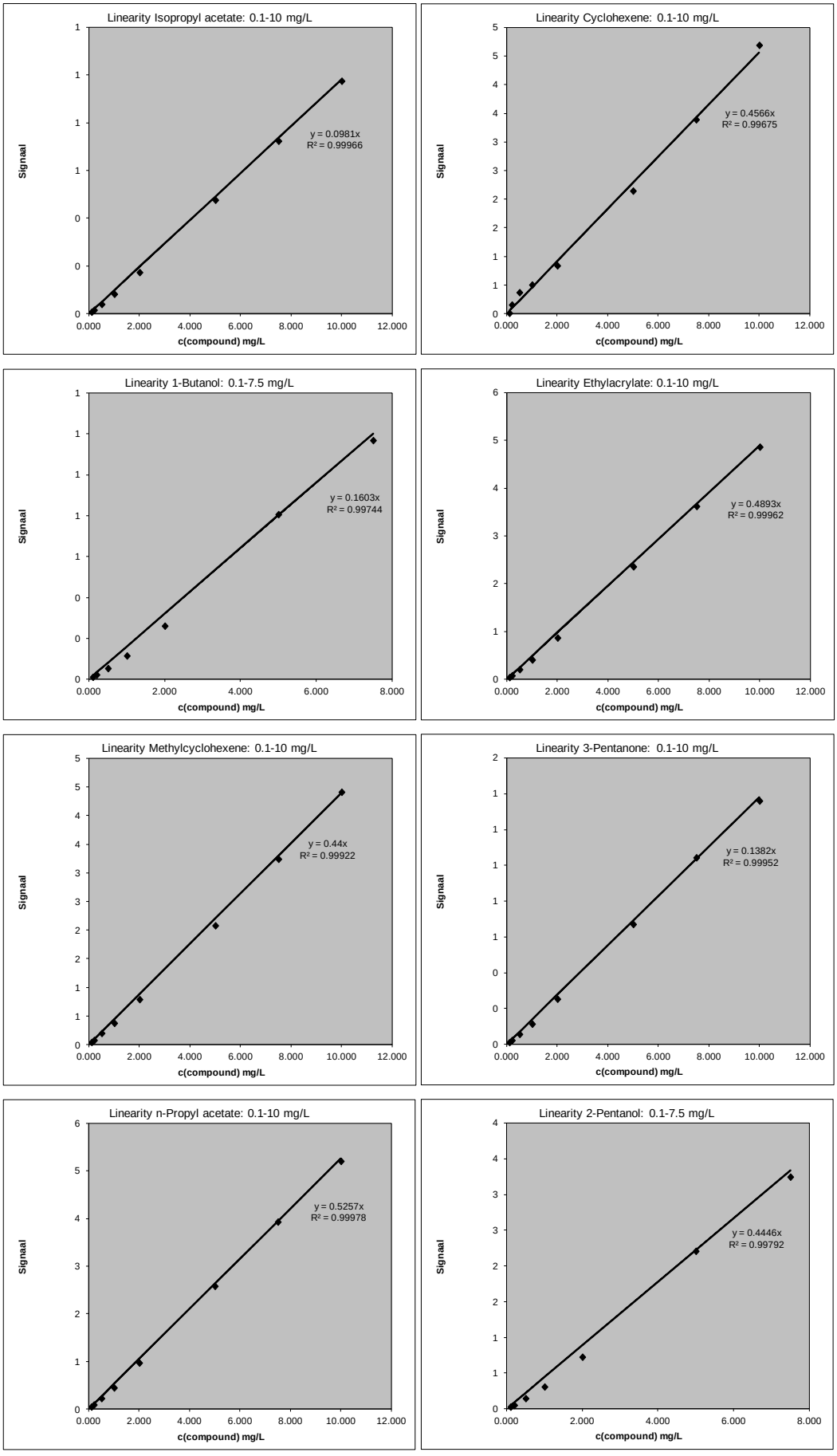
(Figure 2)


Linearity Benzyl acetate: 0.1-10 mg/L
y = 0.3586x
R² = 0.99889
Linearity 1,3-Diisopropylbenzene: 0.1-10 mg/L
y = 0.6431x
R² = 0.99014
Linearity n-Pentane: 0.1-10 mg/L
Linearity Ethanol:0.1-10 mg/L
y = 0.1174x
R² = 0.99548
Linearity Methylal: 0.1-10 mg/L
y = 0.255x
R² = 0.99889
Linearity Acetone: 0.1-7.5 mg/L
y = 0.0719x
R² = 0.99764
Linearity 2-Methylpentane: 0.1-10 mg/L
y = 0.1676x
R² = 0.99838
Linearity tert-Butanol: 0.1-7.5 mg/L
y = 0.3274x
R² = 0.99546
Signaal
c(compound) mg/L

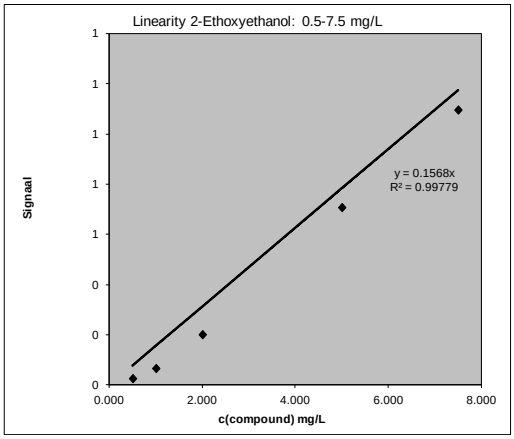
(Figure 2)

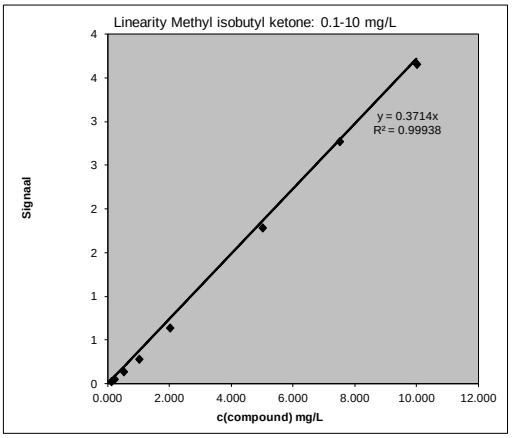

Linearity Allyl alcohol: 0.1-7.5 mg/L
y = 0.1761x
R² = 0.99629
Linearity n-Propanol: 0.1-7.5 mg/L
y = 0.1738x
R² = 0.99734
Linearity Methylcyclopentane: 0.1-10 mg/L
y = 0.3247x
R² = 0.99956
Linearity MEK: 0.1-10 mg/L
y = 0.2401x
R² = 0.99809
Linearity Ethyl acetate: 0.1-10 mg/L
y = 0.3785x
R² = 0.99994
Linearity 2-Butanol: 0.1-7.5 mg/L
y = 0.2628x
R² = 0.99816
Linearity 2-Methyl-1-propanol: 0.1-7.5 mg/L
y = 0.1177x
R² = 0.99815
Linearity Ethylene glycol dimethyl ether: 0.1-10 mg/L
y = 0.7215x
R² = 0.99848
Signaal
c(compound) mg/L

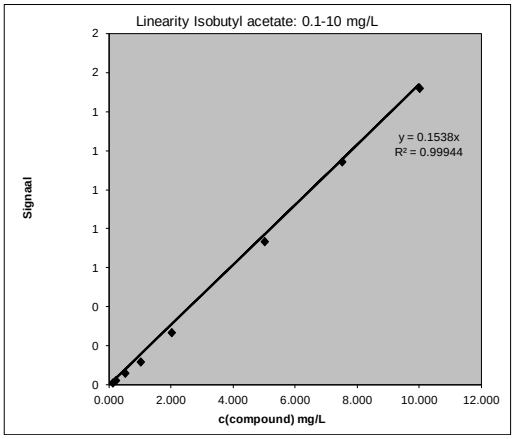
(Figure 2)

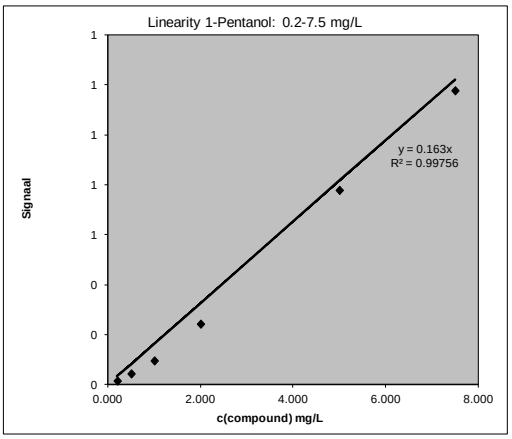

Linearity Isopropyl acetate: 0.1-10 mg/L
y = 0.0981x
R² = 0.99966
Signaal
c(compound) mg/L
Linearity Cyclohexene: 0.1-10 mg/L
y = 0.4566x
R² = 0.99675
Signaal
c(compound) mg/L
Linearity 1-Butanol: 0.1-7.5 mg/L
y = 0.1603x
R² = 0.99744
Signaal
c(compound) mg/L
Linearity Ethylacrylate: 0.1-10 mg/L
y = 0.4893x
R² = 0.99962
Signaal
c(compound) mg/L
Linearity Methylcyclohexene: 0.1-10 mg/L
y = 0.44x
R² = 0.99922
Signaal
c(compound) mg/L
Linearity 3-Pentanone: 0.1-10 mg/L
y = 0.1382x
R² = 0.99952
Signaal
c(compound) mg/L
Linearity n-Propyl acetate: 0.1-10 mg/L
y = 0.5257x
R² = 0.99978
Signaal
c(compound) mg/L
Linearity 2-Pentanol: 0.1-7.5 mg/L
y = 0.4446x
R² = 0.99792
Signaal
c(compound) mg/L

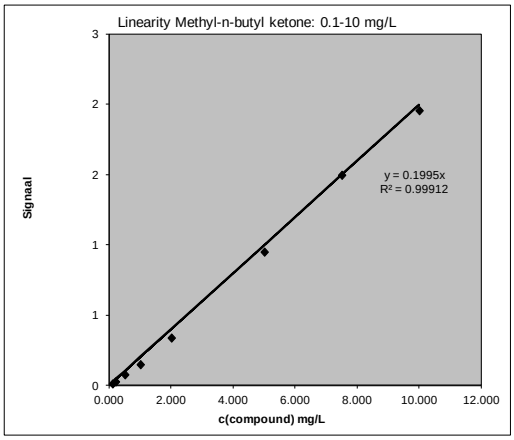
(Figure 2)

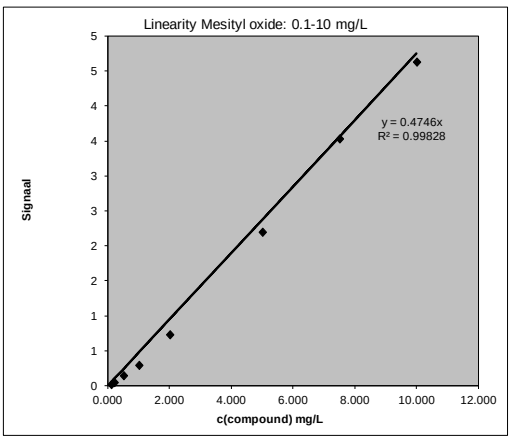

Linearity 2-Ethoxyethanol: 0.5-7.5 mg/L
y = 0.1568x
R² = 0.99779
Signaal
c(compound) mg/L

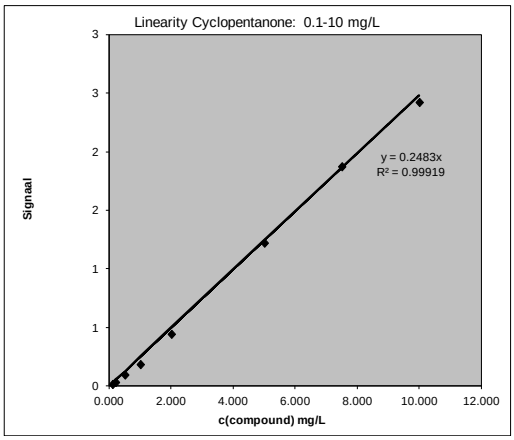

Linearity Methyl isobutyl ketone: 0.1-10 mg/L
y = 0.3714x
R² = 0.99938
Signaal
c(compound) mg/L

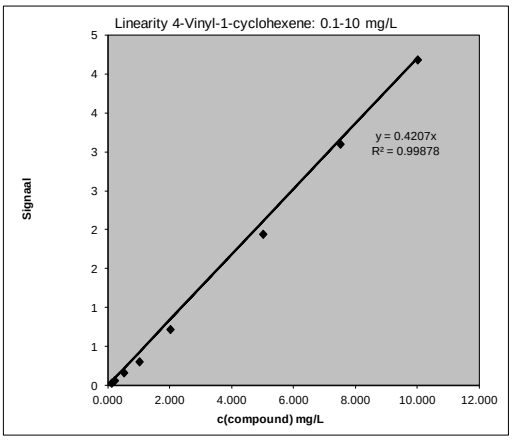

Linearity Isobutyl acetate: 0.1-10 mg/L
y = 0.1538x
R² = 0.99944
Signaal
c(compound) mg/L


Linearity 1-Pentanol: 0.2-7.5 mg/L
y = 0.163x
R² = 0.99756
Signaal
c(compound) mg/L

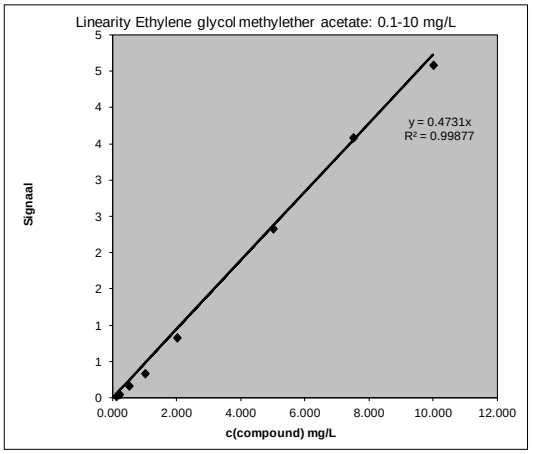

Linearity Methyl-n-butyl ketone: 0.1-10 mg/L
y = 0.1995x
R² = 0.99912
Signaal
c(compound) mg/L

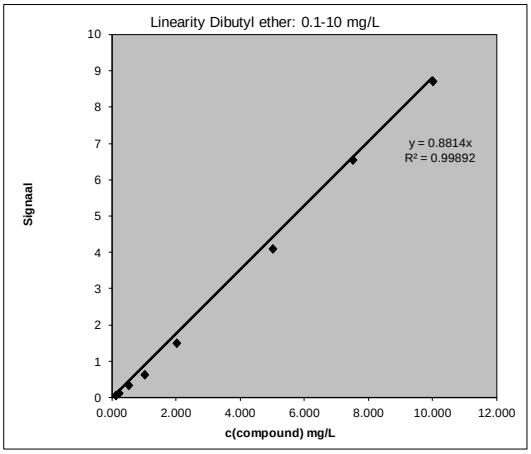

Linearity Mesityl oxide: 0.1-10 mg/L
y = 0.4746x
R² = 0.99828
Signaal
c(compound) mg/L

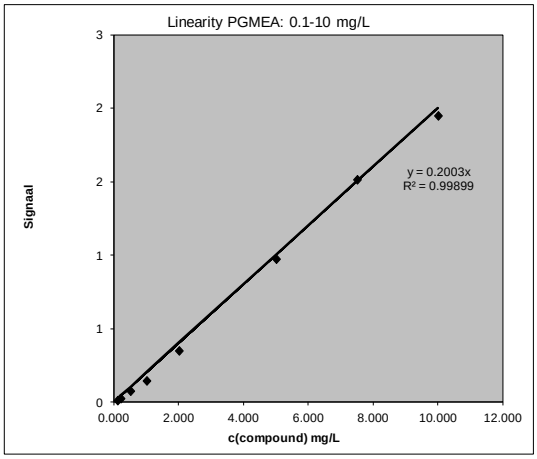

Linearity Cyclopentanone: 0.1-10 mg/L
y = 0.2483x
R² = 0.99919
Signaal
c(compound) mg/L

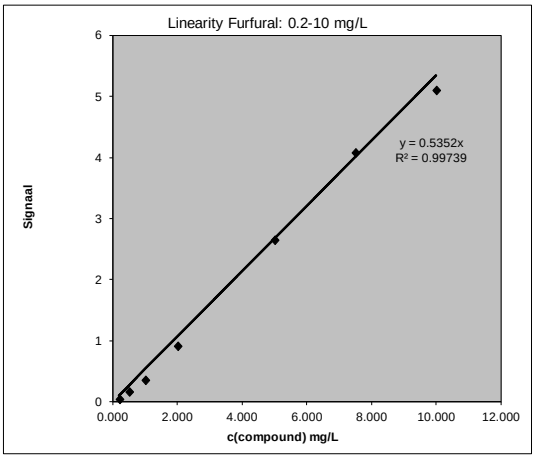

Linearity 4-Vinyl-1-cyclohexene: 0.1-10 mg/L
y = 0.4207x
R² = 0.99878
Signaal
c(compound) mg/L

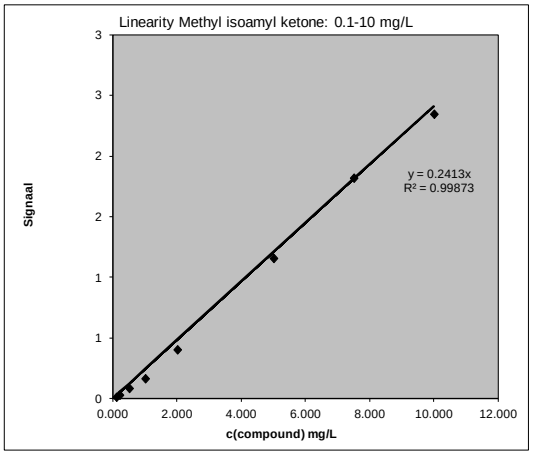
(Figure 2)

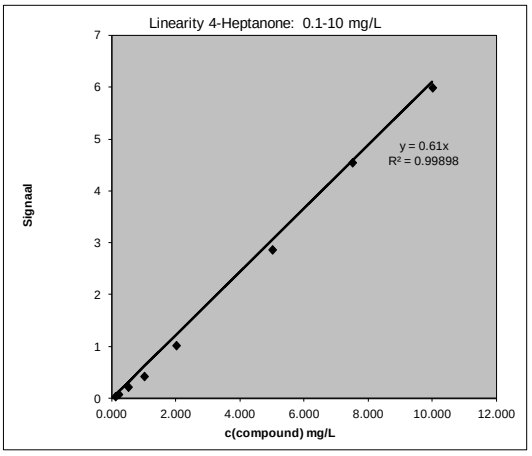

Linearity Ethylene glycol methylether acetate: 0.1-10 mg/L
y = 0.4731x
R² = 0.99877
Signaal
c(compound) mg/L

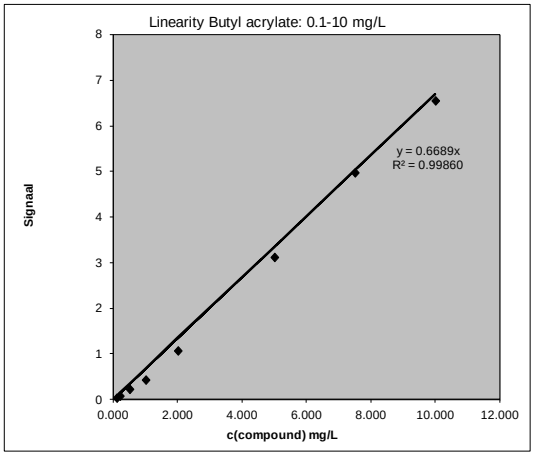

Linearity Dibutyl ether: 0.1-10 mg/L
y = 0.8814x
R² = 0.99892
Signaal
c(compound) mg/L

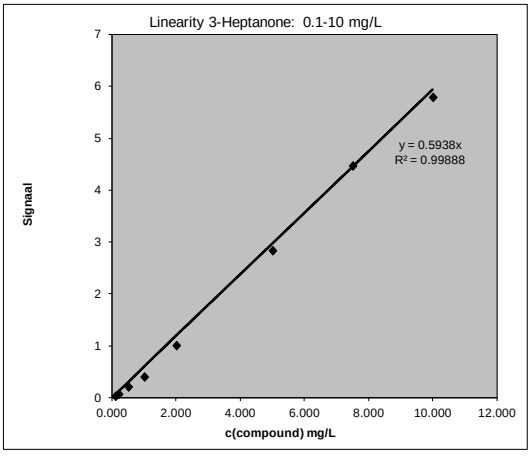

Linearity PGMEA: 0.1-10 mg/L
y = 0.2003x
R² = 0.99899
Signaal
c(compound) mg/L


Linearity Furfural: 0.2-10 mg/L
y = 0.5352x
R² = 0.99739
Signaal
c(compound) mg/L

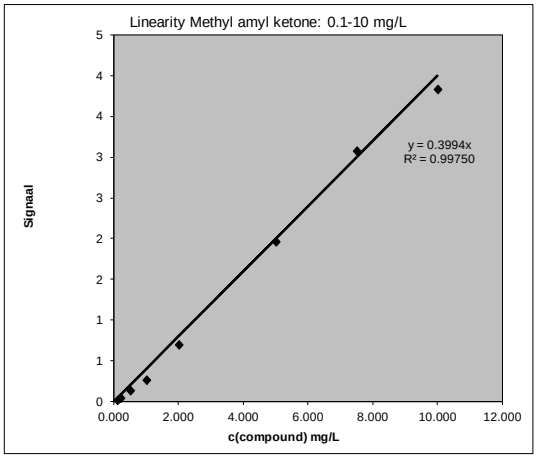

Linearity Methyl isoamyl ketone: 0.1-10 mg/L
y = 0.2413x
R² = 0.99873
Signaal
c(compound) mg/L

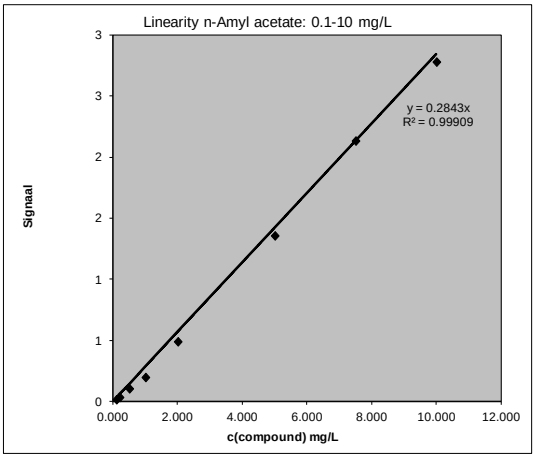

Linearity 4-Heptanone: 0.1-10 mg/L
y = 0.61x
R² = 0.99898
Signaal
c(compound) mg/L

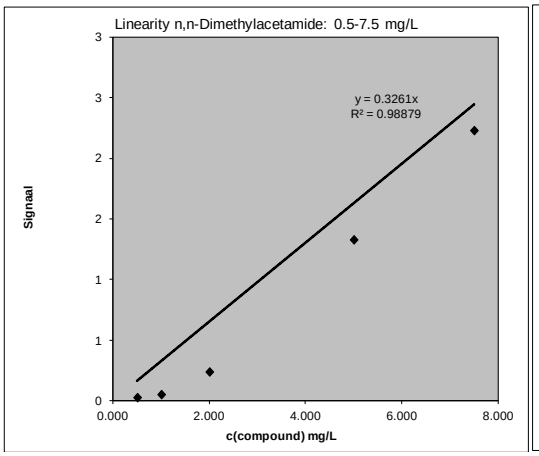

Linearity Butyl acrylate: 0.1-10 mg/L
y = 0.6689x
R² = 0.99860
Signaal
c(compound) mg/L

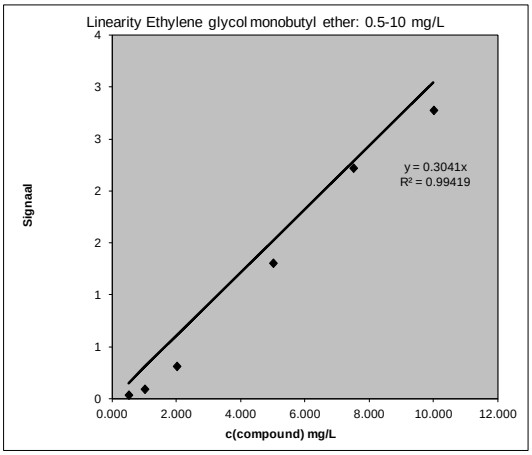

Linearity 3-Heptanone: 0.1-10 mg/L
y = 0.5938x
R² = 0.99888
Signaal
c(compound) mg/L

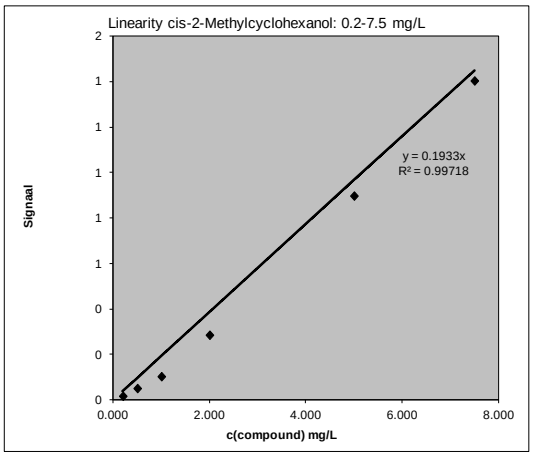
(Figure 2)

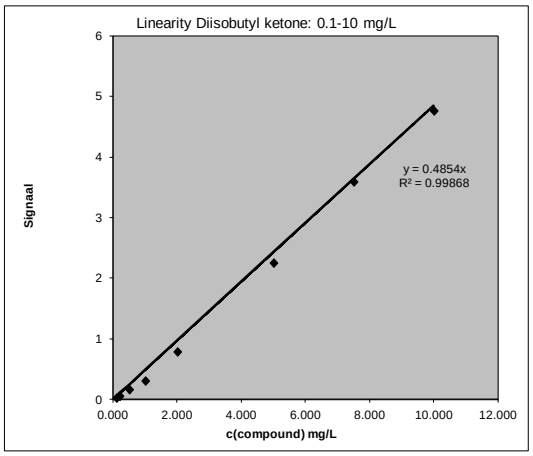

Linearity Methyl amyl ketone: 0.1-10 mg/L
y = 0.3994x
R² = 0.99750
Signaal
c(compound) mg/L

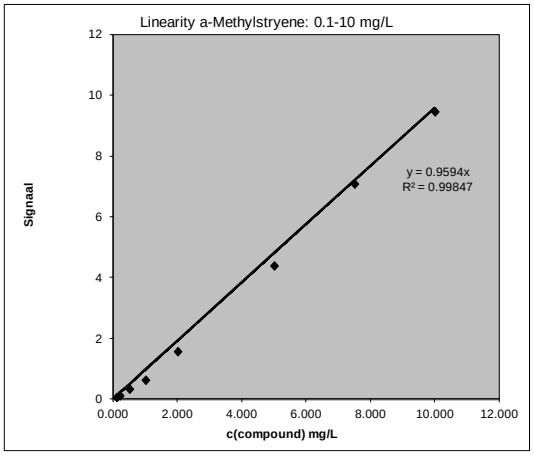

Linearity n-Amyl acetate: 0.1-10 mg/L
y = 0.2843x
R² = 0.99909
Signaal
c(compound) mg/L

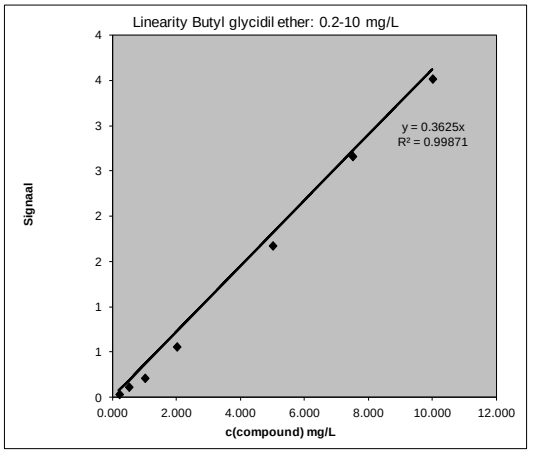

Linearity n,n-Dimethylacetamide: 0.5-7.5 mg/L
y = 0.3261x
R² = 0.98879
Signaal
c(compound) mg/L


Linearity Ethylene glycol monobutyl ether: 0.5-10 mg/L
y = 0.3041x
R² = 0.99419
Signaal
c(compound) mg/L

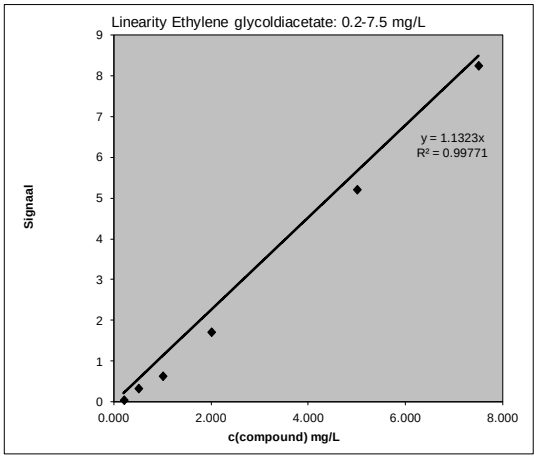

Linearity cis-2-Methylcyclohexanol: 0.2-7.5 mg/L
y = 0.1933x
R² = 0.99718
Signaal
c(compound) mg/L

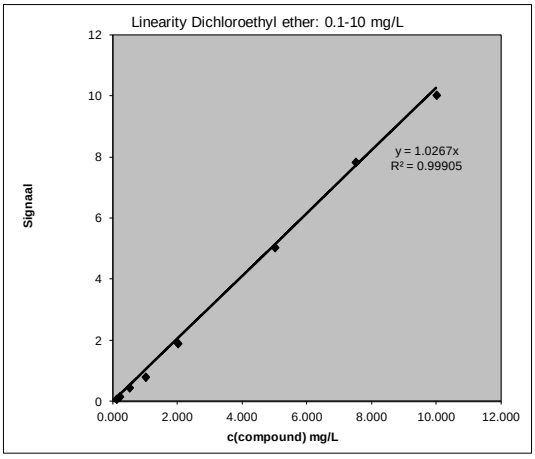

Linearity Diisobutyl ketone: 0.1-10 mg/L
y = 0.4854x
R² = 0.99868
Signaal
c(compound) mg/L

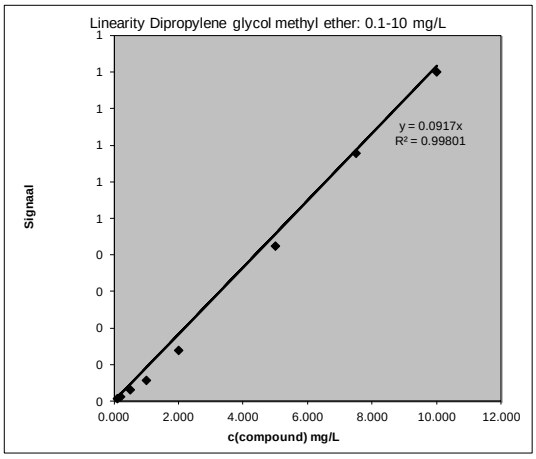

Linearity a-Methylstryene: 0.1-10 mg/L
y = 0.9594x
R² = 0.99847
Signaal
c(compound) mg/L

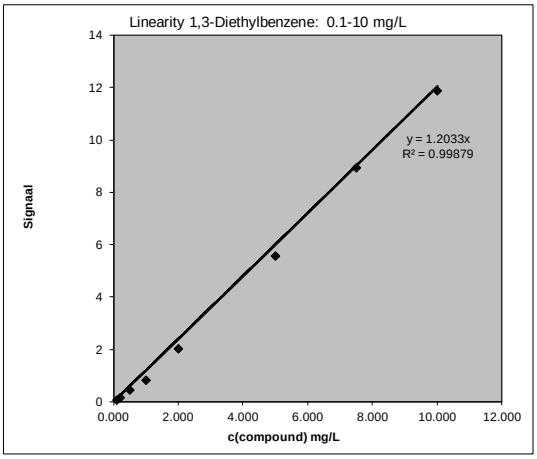

Linearity Butyl glycidil ether: 0.2-10 mg/L
y = 0.3625x
R² = 0.99871
Signaal
c(compound) mg/L

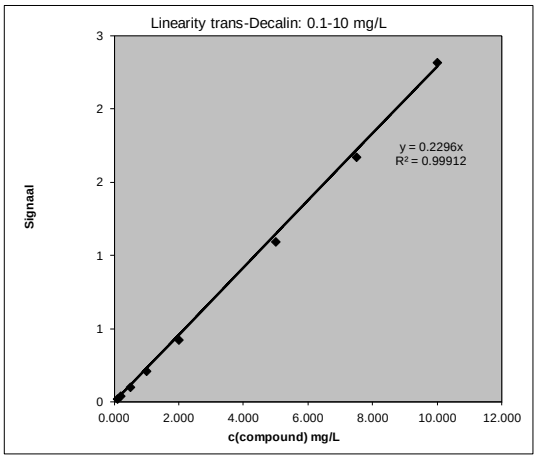
(Figure 2)

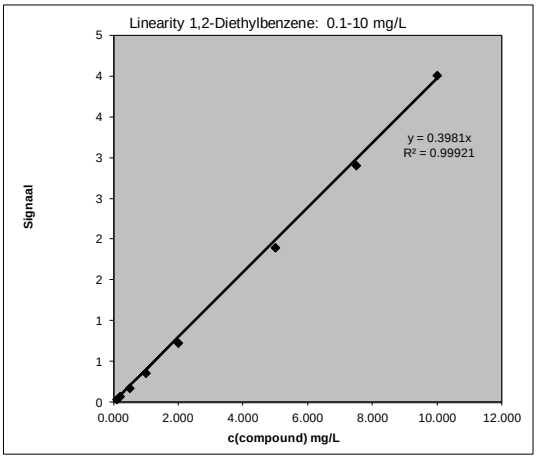

Linearity Ethylene glycoldiacetate: 0.2-7.5 mg/L
y = 1.1323x
R² = 0.99771
Signaal
c(compound) mg/L

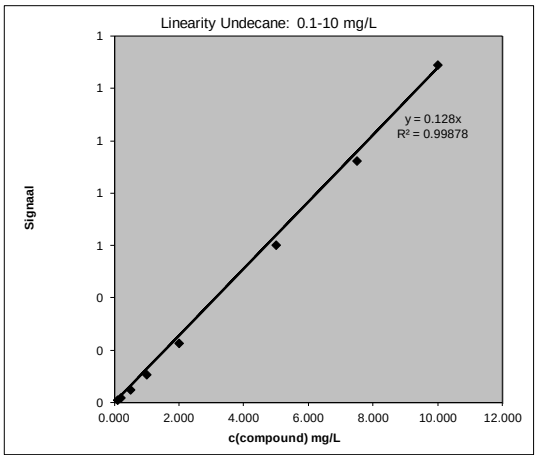

Linearity Dichloroethyl ether: 0.1-10 mg/L
y = 1.0267x
R² = 0.99905
Signaal
c(compound) mg/L

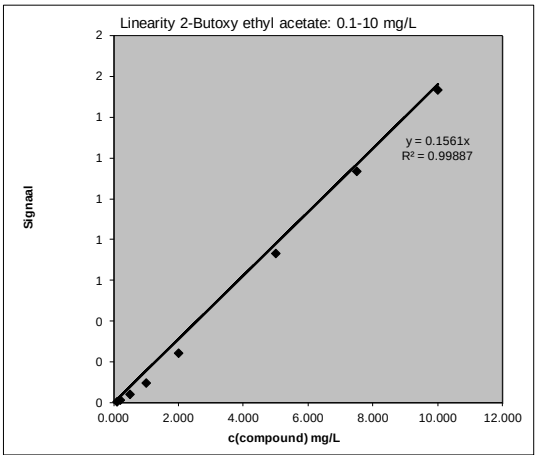

Linearity Dipropylene glycol methyl ether: 0.1-10 mg/L
y = 0.0917x
R² = 0.99801
Signaal
c(compound) mg/L


Linearity 1,3-Diethylbenzene: 0.1-10 mg/L
y = 1.2033x
R² = 0.99879
Signaal
c(compound) mg/L


Linearity trans-Decalin: 0.1-10 mg/L
y = 0.2296x
R² = 0.99912
Signaal
c(compound) mg/L


Linearity 1,2-Diethylbenzene: 0.1-10 mg/L
y = 0.3981x
R² = 0.99921
Signaal
c(compound) mg/L


Linearity Undecane: 0.1-10 mg/L
y = 0.128x
R² = 0.99878
Signaal
c(compound) mg/L


Linearity 2-Butoxy ethyl acetate: 0.1-10 mg/L
y = 0.1561x
R² = 0.99887
Signaal
c(compound) mg/L

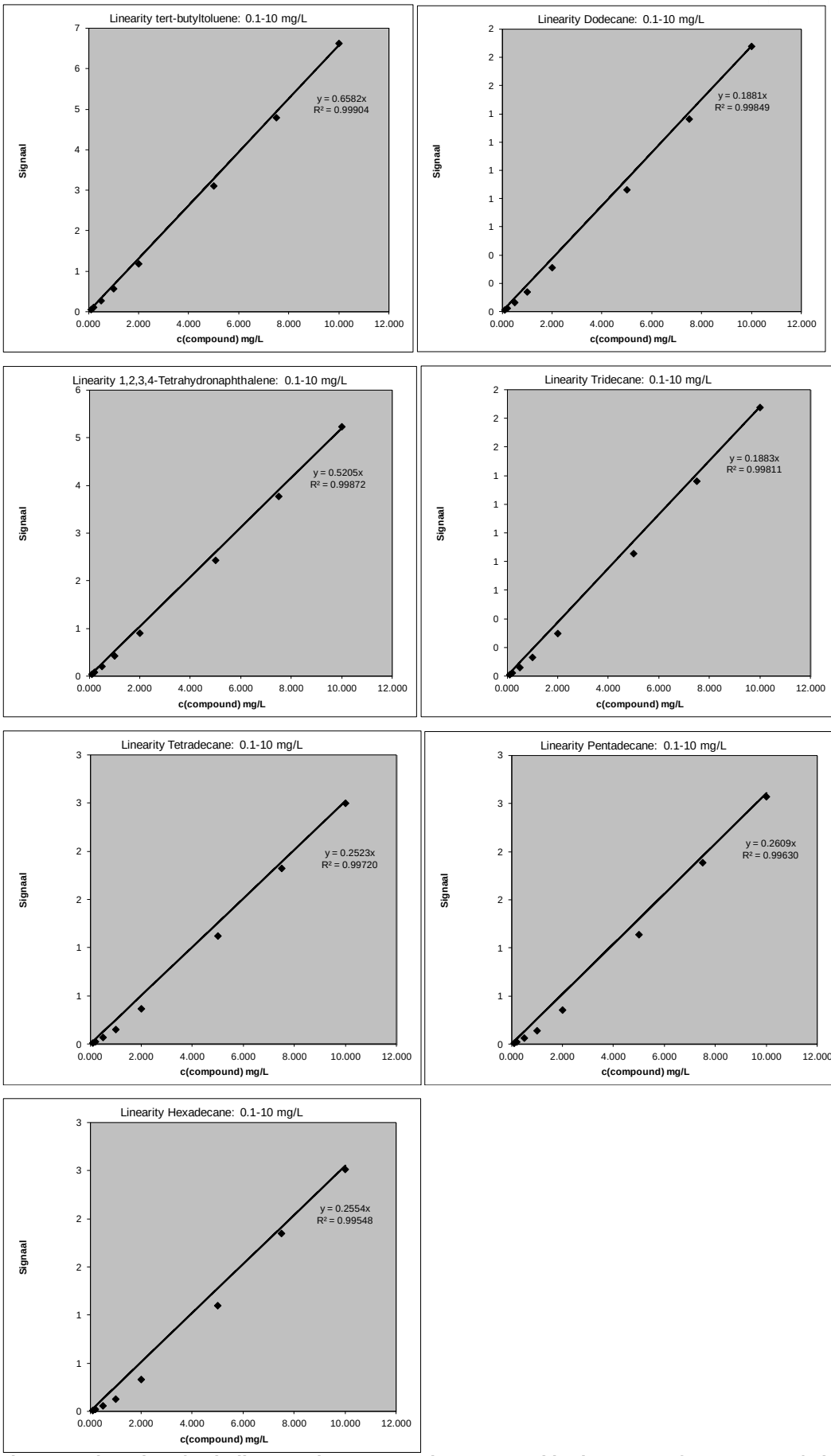


Figure 2. Linearity of volatile organic compounds, measured in the range of 0.1 to 10 mg/L in carbon disulfide. This data was retrieved from measurements on GC-MS system 1.

Table 14. Raw data on the limit of detection and quantitation, measured on the level of 0.1 mg/L with n=8, on GC-MS system 1.

Compound	LOD	LOQ	Variation coefficient %	OK/NOK
1,1,1,2-Tetrachloroethane	0.21	0.42	35.76	NOK
1,1,1-Trichloroethane	0.49	0.99	50.89	NOK
1,1,2,2-Tetrachloroethane	0.05	0.10	18.75	NOK
1,1,2-Trichloro-1,2,2-trifluoroethane	0.64	1.28	57.08	NOK
1,1,2-Trichloroethane	0.19	0.38	36.20	NOK
1,1-Dichloroethane	0.56	1.13	53.81	NOK
1,1-Dichloroethene	0.61	1.22	55.45	NOK
1,1-Dichloropropane	0.41	0.81	46.72	NOK
1,1-Dichloropropene	0.48	0.96	50.21	NOK
1,2,3,4-Tetrahydronaphthalene	0.07	0.15	21.74	NOK
1,2,3-Trichlorobenzene	0.04	0.08	19.75	OK
1,2,3-Trichloropropane	0.08	0.15	22.31	NOK
1,2,3-Trimethylbenzene	0.13	0.26	31.17	NOK
1,2,4-Trichlorobenzene	0.05	0.11	21.03	NOK
1,2,4-Trimethylbenzene	0.15	0.31	34.52	NOK
1,2-Dibromo-3-chloropropane	0.05	0.09	20.32	OK
1,2-Dibromoethane	0.27	0.55	41.65	NOK
1,2-Dichlorobenzene	0.08	0.16	24.95	NOK
1,2-Dichloroethane	0.42	0.84	46.61	NOK
1,2-Dichloropropane	0.38	0.77	46.77	NOK
1,2-Diethylbenzene	0.09	0.18	25.51	NOK
1,3,5-Trichlorobenzene	0.08	0.16	24.54	NOK
1,3,5-Trimethylbenzene	0.18	0.37	35.74	NOK
1,3-Butadiene	0.53	1.05	98.33	NOK
1,3-Dichlorobenzene	0.11	0.22	28.00	NOK
1,3-Dichloropropane	0.27	0.53	41.73	NOK
1,3-Diethylbenzene	0.09	0.17	25.08	NOK
1,3-Diisopropylbenzene	0.02	0.04	23.09	OK
1,4-Dichlorobenzene	0.10	0.20	26.96	NOK
1,4-Diethylbenzene	0.09	0.19	27.44	NOK
1,4-Diisopropylbenzene	0.05	0.10	17.98	NOK
1,4-Dioxane	0.18	0.35	33.25	NOK
1-Bromo-3-chloropropane	0.30	0.59	34.07	NOK
1-Butanol	0.24	0.48	8.27	NOK
1-Methyl-2-pyrrolidone	-	-	-	-
1-Pentanol	0.13	0.26	71.78	NOK
2,2-Dichloropropane	0.65	1.30	53.98	NOK
2,2-Dimethylbutane	0.64	1.29	54.77	NOK
2,3-Dichloropropene	0.42	0.84	49.21	NOK
2,4-Dimethyl-3-pentanone	0.13	0.26	29.74	NOK
2,4-Dimethylpentane	0.42	0.83	49.81	NOK
2-Butanol	0.05	0.10	24.35	OK
2-Butoxy ethyl acetate	0.11	0.22	70.71	NOK
2-Chloro-1,3-butadiene	0.47	0.94	104.26	NOK
2-Chlorotoluene	0.19	0.37	36.50	NOK
2-Ethoxyethanol	-	-	-	-
2-Ethoxyethyl acetate	-	-	-	-
2-Ethyltoluene	0.17	0.33	34.33	NOK
2-Methoxyethanol	0.14	0.27	35.30	NOK
2-Methyl-1-propanol	0.05	0.10	27.19	OK
2-Methyl-2-butanol	0.13	0.25	32.45	NOK
2-Methylbutane	0.30	0.60	27.13	NOK
2-Methylcyclohexanone	0.04	0.07	19.06	OK
2-Methylpentane	0.92	1.84	59.38	NOK
2-Pentanol	0.01	0.02	5.56	OK
2-Propoxyethanol	-	-	-	-
3-Chloro-1-propene (allylchloride)	-	-	-	-
3-Ethyltoluene	0.23	0.46	38.11	NOK
3-Heptanone	0.05	0.11	21.52	NOK
3-methyl-1-Butanol	0.02	0.03	19.88	OK
3-Methyl-2-butanone	0.24	0.49	40.15	NOK
3-Methylcyclohexanone	0.16	0.32	86.60	NOK
3-Pentanol	0.03	0.06	19.16	OK
3-Pentanone	0.19	0.38	37.70	NOK
4-Chlorotoluene	0.16	0.32	34.57	NOK
4-Ethyltoluene	0.19	0.38	36.13	NOK
4-Heptanone	0.06	0.12	22.23	NOK
4-Hydroxy-4-methyl-2-pentanone	-	-	-	-
4-Methylcyclohexanone	-	-	-	-
4-Vinyl-1-cyclohexene	0.30	0.61	42.67	NOK
5-methyl-3-heptanone	0.04	0.08	18.34	OK
Acetone	0.73	1.47	44.48	NOK
Allyl alcohol	0.09	0.18	86.60	NOK
a-Methylstyrene	0.09	0.19	36.95	NOK
a-Pinene	0.25	0.50	37.86	NOK

(Table 14 continuing)

Compound	LOD	LOQ	Variation coefficient %	OK/NOK
Benzene	0.56	1.13	46.37	NOK
Benzyl acetate	0.01	0.03	14.21	OK
Benzyl alcohol	-	-	-	-
Benzyl chloride	0.07	0.14	20.00	NOK
Bromobenzene	0.18	0.36	36.12	NOK
Bromochloromethane	0.47	0.95	51.07	NOK
Bromodichloromethane	0.37	0.74	47.00	NOK
Bromomethane	0.11	0.22	27.47	NOK
Butyl glycidil ether	0.06	0.12	57.88	NOK
Butylacrylate	0.06	0.13	22.28	NOK
Butylbenzene	0.13	0.26	29.58	NOK
Butylmethacrylate	0.04	0.09	21.40	OK
Butylpropionate	0.06	0.12	22.51	NOK
Chloromethane	0.50	1.01	45.22	NOK
cis-1,2-Dichloroethene	0.48	0.97	51.76	NOK
cis-1,3-Dichloropropene	0.29	0.58	42.43	NOK
cis-2-Methylcyclohexanol	-	-	-	-
cis-4-Methylcyclohexanol	0.03	0.06	42.13	OK
cis-Decalin	0.16	0.33	31.93	NOK
Cumene	0.18	0.35	34.04	NOK
Cyclohexane	0.50	1.00	50.34	NOK
Cyclohexanol	0.01	0.02	14.53	OK
Cyclohexanone	0.64	1.27	101.42	NOK
Cyclohexene	0.57	1.13	38.01	NOK
Cyclopentane	0.65	1.31	51.66	NOK
Cyclopentanone	0.09	0.17	45.22	NOK
Dibromochloromethane	0.21	0.42	36.91	NOK
Dibromomethane	0.41	0.83	49.19	NOK
Dibutyl ether	0.14	0.28	33.12	NOK
Dichlorodifluoromethane	0.43	0.85	55.06	NOK
Dichloroethyl ether	0.03	0.06	13.09	OK
Dichloromethane	0.90	1.80	73.59	NOK
Diethylene glycol diethyl ether	-	-	-	-
Diisobutyl ketone	0.05	0.09	22.41	OK
Diisopropylether	0.49	0.98	51.99	NOK
Dimethyl formamide	-	-	-	-
Dipropylene glycol methyl ether	-	-	-	-
D-Limonene	0.13	0.26	31.87	NOK
Dodecane	0.11	0.22	25.64	NOK
EPI	0.23	0.47	35.54	NOK
ETBE	0.45	0.91	50.94	NOK
Ethanol	0.16	0.31	30.48	NOK
Ethyl acetate	0.48	0.96	48.18	NOK
Ethyl propionate	0.30	0.61	47.70	NOK
Ethylacrylate	0.29	0.59	43.91	NOK
Ethylbenzene	0.23	0.45	37.29	NOK
Ethylene chlorohydrin	-	-	-	-
Ethylene glycol diethyl ether	0.04	0.08	22.14	OK
Ethylene glycol dimethyl ether	0.13	0.26	37.06	NOK
Ethylene glycol methylether acetaat	0.10	0.21	87.14	NOK
Ethylene glycol monobutyl ether	-	-	-	-
Ethylene glycoldiacetaat	-	-	-	-
Ethylether	0.62	1.23	54.27	NOK
Ethylmethacrylate	0.20	0.40	39.08	NOK
Furfural	-	-	-	-
Furfuryl alcohol	-	-	-	-
Hexachlorobutadiene	0.08	0.16	21.81	NOK
Hexachloroethaane	0.13	0.26	28.72	NOK
Hexadecane	0.05	0.10	20.92	NOK
Iodomethane	0.19	0.37	52.47	NOK
Isobutyl acetate	0.19	0.38	39.00	NOK
Isobutyl benzene	0.12	0.24	28.79	NOK
Isophorone	0.02	0.04	52.11	OK
Isooctane	-	-	-	-
Isopentyl acetate	0.07	0.14	25.16	NOK
Isopropyl acetate	0.31	0.62	44.83	NOK
Isopropyl glycidil ether	0.03	0.06	15.57	OK
Isopropyl glycol	-	-	-	-
MEK (2-Butanone)	0.30	0.61	44.54	NOK
Mesityl oxide	-	-	-	-
Methacrylonitrile	0.33	0.65	48.70	NOK
Methyl acrylate	0.46	0.92	51.14	NOK
Methyl amyl ketone	0.07	0.13	30.89	NOK
Methyl isoamyl ketone	0.05	0.10	22.96	NOK
Methyl isobutyl carbinol	0.02	0.04	16.09	OK
Methyl isobutyl ketone	0.13	0.25	32.08	NOK
Compound	0.19	0.38	40.16	NOK
Methyl propyl ketone	-	-	-	-

(Table 14 continuing)

Compound	LOD	LOQ	Variation coefficient %	OK/NOK
Methylcyclohexane	-	-	-	-
Methylcyclopentane	0.49	0.98	50.12	NOK
Methylmethacrylate	0.32	0.63	45.04	NOK
Methyl-n-butyl ketone	0.09	0.19	28.57	NOK
Monochlorobenzene	0.21	0.42	36.12	NOK
MTBE	0.57	1.14	55.16	NOK
n,n-Dimethylacetamide	-	-	-	-
Naphthalene	0.06	0.13	22.25	NOK
n-Amyl acetate	0.05	0.09	20.77	OK
n-Butylacetate	0.11	0.21	30.12	NOK
n-Decane	0.27	0.53	40.74	NOK
n-Heptane	0.58	1.15	48.65	NOK
n-Hexane	1.06	2.12	56.73	NOK
n-Nonane	0.36	0.71	45.13	NOK
n-Octane	0.47	0.94	49.02	NOK
n-Pentane	0.44	0.87	17.68	NOK
n-Propanol	0.09	0.17	43.06	NOK
n-Propyl acetate	0.24	0.47	38.25	NOK
o-Xylene	0.19	0.37	34.15	NOK
p,m-Xylene	0.22	0.44	36.69	NOK
Pentachloroethane	0.01	0.02	6.45	OK
Pentadecane	0.04	0.07	15.08	OK
PGME	-	-	-	-
PGMEA	0.07	0.14	51.87	NOK
p-isopropyltoluene	-	-	-	-
Propylbenzene	0.19	0.39	35.82	NOK
sec-Butylbenzene	0.15	0.31	32.50	NOK
Styrene	0.13	0.25	40.49	NOK
TAME	0.46	0.91	49.63	NOK
tert-Butanol	0.15	0.31	48.98	NOK
tert-Butylbenzene	0.16	0.32	32.27	NOK
tert-Butyltoluene	0.07	0.14	21.06	NOK
Tetrachloroethene	0.43	0.87	40.40	NOK
Tetrachloromethane	0.47	0.95	49.26	NOK
Tetradecane	0.06	0.13	17.31	NOK
THF (tetrahydrofuran)	0.33	0.67	45.68	NOK
THT (tetrahydrothiofeen)	0.15	0.30	43.92	NOK
Toluene	0.32	0.64	36.94	NOK
trans-1,2-Dichloroethene	0.62	1.23	56.45	NOK
trans-1,3-Dichloropropene	0.22	0.44	37.64	NOK
trans-2-Methylcyclohexanol	0.27	0.54	55.74	NOK
trans-4-Methylcyclohexanol	-	-	-	-
trans-Decalin	0.19	0.39	34.62	NOK
Tribromomethane	0.08	0.17	25.11	NOK
Trichloroethene	0.45	0.89	48.32	NOK
Trichloromethane	0.45	0.90	49.34	NOK
Trichloromonofluoromethane	0.54	1.08	46.60	NOK
Tridecane	0.05	0.09	20.24	OK
Undecane	0.15	0.29	35.61	NOK
Vinylchloride	0.50	1.00	51.83	NOK

Table 15. Raw data on the reproducibility with n=8, measured on the level of 2 mg/L, on GC-MS system 1.

Compound	1	2	3	4	5	6	7	8	Variation coefficient %	OK/NOK
1,1,1,2-Tetrachloroethane	2.03	1.96	1.96	1.86	1.83	1.95	1.91	1.95	**3.14**	OK
1,1,1-Trichloroethane	2.03	1.95	1.92	1.85	1.80	1.98	1.94	1.99	**4.04**	OK
1,1,2,2-Tetrachloroethane	1.28	1.29	1.22	1.17	1.21	1.37	1.17	1.32	**6.25**	OK
1,1,2-Trichloro-1,2,2-trifluoroethane	2.04	1.65	1.98	1.11	2.03	1.80	2.32	2.17	**21.86**	NOK
1,1,2-Trichloroethane	1.94	1.94	1.78	2.06	1.75	1.86	1.74	1.79	**5.73**	OK
1,1-Dichloroethane	1.87	1.81	1.92	1.50	1.79	1.85	1.97	1.99	**8.78**	OK
1,1-Dichloroethene	1.93	1.73	1.91	1.25	1.94	1.72	2.14	2.14	**15.86**	OK
1,1-Dichloropropane	1.97	1.96	1.88	1.91	1.76	1.93	1.88	1.95	**3.62**	OK
1,1-Dichloropropene	1.97	1.95	1.87	1.87	1.79	1.95	1.88	1.97	**3.40**	OK
1,2,3,4-Tetrahydronaphthalene	2.22	2.46	1.97	2.77	2.19	2.47	2.12	2.22	**13.25**	OK
1,2,3-Trichlorobenzene	1.21	1.38	1.13	1.59	1.33	1.54	1.26	1.40	**14.37**	OK
1,2,3-Trichloropropane	1.79	1.91	1.68	2.22	1.81	1.90	1.71	1.81	**10.30**	OK
1,2,3-Trimethylbenzene	1.79	1.88	1.79	1.87	1.74	1.93	1.81	1.85	**4.39**	OK
1,2,4-Trichlorobenzene	1.43	1.61	1.32	1.85	1.49	1.68	1.42	1.52	**13.34**	OK
1,2,4-Trimethylbenzene	1.90	1.96	1.88	1.96	1.83	2.03	1.92	1.95	**4.14**	OK
1,2-Dibromo-3-chloropropane	1.41	1.44	1.29	1.49	1.65	1.81	1.66	1.83	**6.95**	OK
1,2-Dibromoethane	1.97	1.93	1.92	1.84	1.76	1.94	1.90	1.94	**3.93**	OK
1,2-Dichlorobenzene	1.64	1.79	1.53	2.07	1.63	1.81	1.53	1.64	**11.87**	OK
1,2-Dichloroethane	1.90	1.92	1.84	1.73	1.73	1.89	1.86	1.88	**3.73**	OK
1,2-Dichloropropane	2.03	2.00	1.87	1.97	1.79	1.92	1.83	1.92	**3.62**	OK
1,2-Diethylbenzene	2.00	2.21	1.84	2.49	1.91	2.09	1.82	1.91	**11.84**	OK
1,3,5-Trichlorobenzene	1.68	1.85	1.56	2.10	1.65	1.86	1.56	1.66	**12.12**	OK
1,3,5-Trimethylbenzene	1.96	2.04	1.95	2.00	1.86	2.07	1.94	1.97	**4.06**	OK
1,3-Butadiene	1.70	1.67	1.57	1.13	1.18	1.10	1.40	1.50	**12.04**	OK
1,3-Dichlorobenzene	1.79	1.94	1.66	2.22	1.73	1.88	1.61	1.72	**11.28**	OK
1,3-Dichloropropane	2.00	2.02	2.02	2.12	1.81	1.92	1.74	1.81	**3.02**	OK
1,3-Diethylbenzene	2.09	2.33	1.89	2.57	1.97	2.17	1.90	1.98	**11.97**	OK
1,3-Diisopropylbenzene	1.53	1.83	1.16	2.06	1.59	1.63	1.59	2.00	**22.33**	NOK
1,4-Dichlorobenzene	1.74	1.89	1.60	2.17	1.68	1.86	1.58	1.69	**11.82**	OK
1,4-Diethylbenzene	2.10	2.31	1.89	2.55	1.95	2.14	1.89	1.95	**11.52**	OK
1,4-Diisopropylbenzene	2.20	2.43	1.96	2.71	2.05	2.35	2.03	2.08	**12.75**	OK
1,4-Dioxane	2.22	2.11	2.06	2.23	2.16	2.34	2.25	2.31	**4.43**	OK
1-Bromo-3-chloropropane	3.92	4.12	3.57	4.57	3.68	3.87	3.54	3.69	**9.13**	OK
1-Butanol	1.27	1.24	1.05	1.25	2.19	2.18	2.34	2.34	**6.23**	OK
1-Methyl-2-pyrrolidone	-	-	-	-	-	-	-	-	**-**	-
1-Pentanol	0.90	0.80	0.64	1.00	1.23	1.20	1.24	1.26	**16.20**	OK
2,2-Dichloropropane	1.95	1.86	2.00	1.38	1.77	1.93	2.02	1.98	**13.42**	OK
2,2-Dimethylbutane	2.02	1.79	1.97	1.32	1.85	1.77	2.14	2.22	**14.86**	OK
2,3-Dichloropropene	1.90	1.81	1.95	1.59	1.73	1.89	1.96	1.95	**8.07**	OK
2,4-Dimethyl-3-pentanone	2.07	2.12	1.88	2.25	1.89	1.96	1.87	1.95	**6.72**	OK
2,4-Dimethylpentane	1.77	1.76	1.63	1.51	1.60	1.71	1.70	1.74	**3.79**	OK
2-Butanol	0.99	0.92	0.92	0.91	1.08	1.04	1.16	1.16	**2.87**	OK
2-Butoxy ethyl acetate	0.72	0.78	0.50	1.06	1.84	1.99	1.78	2.24	**26.67**	NOK
2-Chloro-1,3-butadiene	1.61	1.61	1.54	1.36	1.36	1.36	1.46	1.51	**4.54**	OK
2-Chlorotoluene	1.81	1.87	1.80	1.83	1.72	1.90	1.80	1.83	**3.82**	OK
2-Ethoxyethanol	0.58	0.56	0.43	0.78	1.08	1.06	1.11	1.25	**21.35**	NOK
2-Ethoxyethyl acetate	1.07	1.04	0.73	1.39	2.22	2.16	2.18	2.22	**22.13**	NOK
2-Ethyltoluene	1.91	1.97	1.90	1.96	1.83	2.01	1.90	1.94	**3.83**	OK
2-Methoxyethanol	2.08	2.02	1.80	1.86	1.76	1.90	1.94	1.84	**3.63**	OK
2-Methyl-1-propanol	0.85	0.83	0.75	0.84	1.00	0.99	1.07	1.04	**4.22**	OK
2-Methyl-2-butanol	1.16	1.13	1.13	1.12	1.29	1.30	1.37	1.44	**2.19**	OK
2-Methylbutane	1.34	1.72	1.45	1.48	1.11	1.05	1.13	1.40	**11.81**	OK
2-Methylcyclohexanone	1.47	1.57	1.27	2.39	2.36	2.50	2.79	2.75	**21.82**	NOK
2-Methylpentane	1.41	1.57	1.78	1.19	1.50	1.54	1.65	1.84	**15.12**	OK
2-Pentanol	0.98	0.95	0.84	1.02	1.19	1.19	1.27	1.32	**6.93**	OK
2-Propoxyethanol	0.58	0.56	0.35	0.83	1.51	1.47	1.40	1.68	**29.13**	NOK
3-Chloro-1-propene (allylchloride)	-	-	-	-	-	-	-	-	**-**	-
3-Ethyltoluene	2.00	2.04	1.98	2.01	1.89	2.07	1.98	2.02	**3.51**	OK
3-Heptanone	2.03	2.12	1.78	2.49	2.02	2.09	2.02	2.11	**12.01**	OK
3-methyl-1-Butanol	0.74	0.72	0.59	0.78	1.03	1.05	1.07	1.18	**10.59**	OK
3-Methyl-2-butanone	1.95	1.94	1.91	1.83	1.73	1.89	1.97	1.97	**3.56**	OK
3-Methylcyclohexanone	1.13	1.20	0.93	-	3.82	4.78	7.26	3.07	**53.37**	NOK
3-Pentanol	1.11	1.05	0.95	1.15	1.30	1.32	1.33	1.40	**7.44**	OK
3-Pentanone	2.01	2.05	1.88	1.96	1.79	1.98	2.02	1.99	**3.89**	OK
4-Chlorotoluene	1.81	1.86	1.82	1.86	1.75	1.92	1.82	1.85	**3.53**	OK
4-Ethyltoluene	2.00	2.06	2.00	2.02	1.88	2.07	1.96	1.99	**3.55**	OK
4-Heptanone	2.04	2.11	1.80	2.41	1.97	2.01	1.93	2.02	**10.42**	OK
4-Hydroxy-4-methyl-2-pentanone	-	-	-	-	0.63	0.74	0.63	1.11	**28.77**	NOK
4-Methylcyclohexanone	1.10	1.18	0.87	-	3.24	-	-	3.14	**86.67**	NOK
4-Vinyl-1-cyclohexene	2.20	2.31	1.95	2.46	2.01	2.09	1.93	2.08	**8.90**	OK
5-methyl-3-heptanone	1.92	2.06	1.68	2.39	1.95	1.99	1.85	1.98	**12.96**	OK
Acetone	1.59	1.34	1.81	0.80	1.22	0.98	1.32	1.14	**29.48**	NOK
Allyl alcohol	0.70	0.57	0.63	0.59	0.66	0.54	0.67	0.68	**10.39**	OK
a-Methylstyrene	2.14	2.32	1.80	2.53	1.84	1.94	1.85	1.97	**12.64**	OK
a-Pinene	2.25	2.42	2.01	2.66	2.07	2.21	1.99	2.11	**10.70**	OK

(Table 15 continuing)

Compound	1	2	3	4	5	6	7	8	Variation coefficient %	OK/NOK
Benzene	1.35	1.35	1.32	1.84	1.74	1.83	1.79	1.88	**12.01**	OK
Benzyl acetate	0.84	0.89	0.58	1.20	2.00	2.16	1.93	2.39	**25.71**	NOK
Benzyl alcohol	0.18	0.22	-	0.33	0.71	0.76	0.71	0.91	**37.31**	NOK
Benzyl chloride	2.65	2.74	2.16	3.33	2.70	2.72	2.39	2.54	**15.25**	OK
Bromobenzene	1.80	1.84	1.79	1.86	1.75	1.87	1.77	1.85	**3.20**	OK
Bromochloromethane	1.83	1.82	1.79	1.61	1.68	1.85	1.88	1.88	**5.09**	OK
Bromodichloromethane	1.85	1.80	1.91	1.59	1.69	1.84	1.92	1.90	**7.30**	OK
Bromomethane	1.04	1.13	0.58	0.72	0.58	0.61	0.65	0.74	**9.33**	OK
Butyl glycidil ether	1.34	1.43	1.06	1.84	2.13	2.20	2.00	2.27	**19.66**	OK
Butylacrylate	2.34	2.42	1.95	2.66	2.11	2.17	2.00	2.14	**11.26**	OK
Butylbenzene	2.00	2.10	1.99	2.06	1.89	2.14	1.99	2.00	**4.98**	OK
Butylmethacrylate	2.35	2.45	1.91	2.72	2.19	2.27	1.97	2.17	**12.88**	OK
Butylpropionate	2.34	2.34	1.99	2.69	2.15	2.24	2.03	2.17	**10.96**	OK
Chloroethane	1.78	1.84	1.44	1.39	1.32	1.35	1.43	1.55	**3.25**	OK
Chloromethane	1.30	1.02	0.28	0.34	0.51	1.50	1.03	1.17	**36.81**	NOK
cis-1,2-Dichloroethene	1.82	1.79	1.87	1.57	1.69	1.79	1.87	1.90	**6.70**	OK
cis-1,3-Dichloropropene	2.00	2.01	1.82	2.07	1.80	1.89	1.79	1.87	**5.19**	OK
cis-2-Methylcyclohexanol	0.72	0.74	0.49	0.98	1.38	1.35	1.27	1.62	**25.00**	NOK
cis-4-Methylcyclohexanol	0.73	0.76	0.50	0.87	1.28	1.20	1.05	1.37	**21.39**	NOK
cis-Decalin	2.30	2.58	2.11	2.83	2.13	2.39	2.04	2.16	**11.92**	OK
Cumene	2.07	2.22	1.87	2.48	1.95	2.08	1.85	1.96	**10.61**	OK
Cyclohexane	1.98	1.97	1.91	1.82	1.77	1.93	1.87	1.97	**3.94**	OK
Cyclohexanol	0.42	0.47	0.31	0.59	1.05	1.05	1.01	1.41	**25.11**	NOK
Cyclohexanone	1.23	1.29	1.05	-	5.19	7.11	11.08	3.60	**59.71**	NOK
Cyclohexene	1.70	1.79	1.51	1.69	1.56	1.52	1.32	1.84	**12.54**	OK
Cyclopentane	1.44	1.66	1.87	1.25	1.62	1.71	1.84	2.02	**15.19**	OK
Cyclopentanone	1.63	1.58	1.45	2.20	1.86	2.08	2.36	2.10	**15.62**	OK
Dibromochloromethane	1.93	1.88	1.85	1.78	1.75	1.89	1.90	1.90	**3.05**	OK
Dibromomethane	1.81	1.75	1.87	1.55	1.68	1.89	1.97	1.92	**7.89**	OK
Dibutyl ether	2.06	2.16	1.83	2.41	1.91	1.97	1.81	1.90	**10.05**	OK
Dichlorodifluoromethane	1.25	1.18	0.62	0.28	0.43	1.84	1.36	1.02	**52.21**	NOK
Dichloroethyl ether	2.02	2.15	1.78	2.65	2.75	2.96	2.62	2.80	**14.61**	OK
Dichloromethane	1.68	1.62	1.87	1.17	1.79	1.68	2.04	1.48	**19.83**	OK
Diethylene glycol diethyl ether	0.26	0.31	0.18	0.48	1.34	1.43	1.52	2.13	**34.55**	NOK
Diisobutyl ketone	1.92	2.10	1.70	2.40	1.97	2.04	1.82	1.98	**12.91**	OK
Diisopropylether	1.94	1.90	1.96	1.71	1.82	1.90	1.97	2.02	**5.25**	OK
Dimethyl formamide	-	-	-	-	-	-	-	-	**-**	-
Dipropylene glycol methyl ether	-	-	-	-	-	-	-	-	**-**	-
D-Limonene	2.40	2.57	2.03	2.78	2.07	2.25	2.01	2.12	**11.81**	OK
Dodecane	2.27	2.52	1.93	2.66	1.90	2.22	1.98	2.01	**13.12**	OK
EPI	2.65	2.62	2.47	2.63	2.35	2.52	2.46	2.51	**3.51**	OK
ETBE	1.99	1.95	1.99	1.78	1.82	1.95	1.96	2.01	**4.72**	OK
Ethanol	0.67	0.48	0.61	0.52	0.72	0.46	0.70	0.57	**21.59**	NOK
Ethyl acetate	2.19	2.16	2.35	1.94	2.07	2.09	2.22	2.17	**6.68**	OK
Ethyl propionate	2.33	2.23	2.08	2.21	2.00	2.15	2.11	2.23	**4.26**	OK
Ethylacrylate	2.33	2.29	2.18	2.28	2.07	2.19	2.18	2.26	**2.91**	OK
Ethylbenzene	2.05	2.17	1.86	2.41	1.95	2.02	1.84	1.93	**9.62**	OK
Ethylene chlorohydrin	0.44	0.44	1.08	0.45	0.59	0.52	0.60	0.57	**29.66**	NOK
Ethylene glycol diethyl ether	1.91	1.93	1.68	2.19	1.98	2.01	1.95	2.04	**9.56**	OK
Ethylene glycol dimethyl ether	1.87	1.76	1.62	1.69	1.59	1.73	1.75	1.66	**4.43**	OK
Ethylene glycol methylether acetaat	1.49	1.38	1.08	1.71	2.24	2.28	2.17	2.36	**16.41**	OK
Ethylene glycol monobutyl ether	-	-	-	1.44	4.54	3.87	4.09	-	**71.15**	NOK
Ethylene glycoldiacetaat	0.59	0.51	0.31	0.77	2.16	2.26	2.14	2.45	**30.63**	NOK
Ethylether	2.08	1.72	1.97	1.37	2.10	1.76	2.24	2.16	**15.75**	OK
Ethylmethacrylate	2.06	1.96	1.93	1.78	1.80	1.94	2.01	2.04	**4.41**	OK
Furfural	1.21	1.21	0.97	2.70	2.52	2.64	3.20	2.09	**36.43**	NOK
Furfuryl alcohol	1.28	1.23	0.59	1.58	1.75	1.62	1.27	1.11	**32.67**	NOK
Hexachlorobutadiene	1.71	1.86	1.77	1.86	1.76	2.09	1.87	1.85	**6.92**	OK
Hexachloroethaane	1.80	1.88	1.89	1.89	1.75	2.04	1.86	1.87	**5.63**	OK
Hexadecane	1.91	2.30	1.74	2.57	1.93	2.48	2.15	1.87	**18.14**	OK
Iodomethane	1.23	1.19	1.00	0.87	1.06	0.98	1.15	1.18	**5.88**	OK
Isobutyl acetate	2.37	2.30	2.01	2.41	2.07	2.12	2.08	2.21	**6.90**	OK
Isobutyl benzene	2.20	2.38	1.99	2.69	2.07	2.26	1.96	2.07	**11.52**	OK
Isophorone	0.28	0.34	0.22	0.45	0.74	0.83	0.73	1.23	**31.68**	NOK
Isooctane	-	-	-	-	-	-	-	-	**-**	-
Isopentyl acetate	2.32	2.28	1.97	2.58	2.10	2.24	2.03	2.16	**10.03**	OK
Isopropyl acetate	2.27	2.24	2.14	2.04	2.00	2.14	2.18	2.13	**2.91**	OK
Isopropyl glycidil ether	1.62	1.62	1.32	1.97	2.08	2.11	1.94	2.17	**14.47**	OK
Isopropyl glycol	0.41	0.41	0.25	0.53	1.19	1.02	1.24	1.50	**26.84**	NOK
MEK (2-Butanone)	1.91	1.82	1.91	1.65	1.72	1.78	2.06	1.97	**5.77**	OK
Mesityl oxide	-	-	-	-	-	-	-	-	**-**	-
Methacrylonitrile	1.82	1.70	1.82	1.59	1.67	1.72	1.86	1.84	**5.53**	OK
Methyl acrylate	2.27	2.15	2.26	1.99	2.10	2.13	2.29	2.27	**4.90**	OK
Methyl amyl ketone	1.84	1.95	1.55	2.52	2.10	2.07	2.35	2.35	**16.87**	OK
Methyl isoamyl ketone	1.92	1.95	1.67	2.49	1.98	2.02	2.24	2.21	**14.01**	OK
Methyl isobutyl carbinol	1.01	0.96	0.82	1.09	1.30	1.29	1.24	1.43	**11.34**	OK
Methyl isobutyl ketone	2.03	2.06	1.82	2.07	1.80	1.89	1.89	1.91	**4.95**	OK

(Table 15 continuing)

Compound	1	2	3	4	5	6	7	8	Variation coefficient %	OK/NOK
Methyl propyl ketone	2.01	1.99	1.95	1.99	1.72	1.90	2.15	1.99	**4.50**	OK
Methylal	-	-	-	-	-	-	-	-	**-**	-
Methylcyclohexane	-	-	-	-	-	-	-	-	**-**	-
Methylcyclopentane	1.84	1.84	1.71	1.64	1.69	1.81	1.83	1.96	**3.91**	OK
Methylmethacrylate	2.01	1.85	2.00	1.59	1.73	1.89	2.01	1.92	**9.18**	OK
Methyl-n-butyl ketone	2.21	2.24	1.93	2.56	2.07	2.12	2.40	2.32	**10.15**	OK
Monochlorobenzene	1.85	1.96	1.76	2.18	1.76	1.87	1.65	1.80	**8.68**	OK
MTBE	1.88	1.85	2.05	1.60	1.87	1.89	2.05	2.04	**8.89**	OK
n,n-Dimethylacetamide	-	-	-	-	-	-	-	-	**-**	-
Naphthalene	1.38	1.38	1.33	1.41	1.64	1.76	1.68	1.78	**3.88**	OK
n-Amyl acetate	2.28	2.32	1.94	2.65	2.16	2.22	2.08	2.23	**11.13**	OK
n-Butylacetate	2.30	2.31	2.01	2.56	2.11	2.17	2.05	2.14	**8.60**	OK
n-Decane	2.12	2.23	2.13	2.16	1.96	2.16	2.04	2.10	**4.05**	OK
n-Heptane	2.03	1.98	1.97	1.64	1.78	1.98	1.98	2.10	**7.92**	OK
n-Hexane	1.99	2.04	2.37	1.66	1.83	1.92	2.00	1.52	**15.89**	OK
n-Nonane	2.06	2.06	1.99	2.02	1.90	2.05	1.98	2.08	**3.22**	OK
n-Octane	2.04	2.00	2.00	1.86	1.88	2.01	1.97	2.06	**3.88**	OK
n-Pentane	0.83	0.73	0.89	0.66	0.96	0.75	1.01	0.91	**15.20**	OK
n-Propanol	0.85	0.76	0.72	0.75	0.87	0.82	0.97	0.85	**6.84**	OK
n-Propyl acetate	2.27	2.21	2.16	2.26	2.05	2.16	2.11	2.14	**2.64**	OK
o-Xylene	1.94	2.06	1.78	2.34	1.83	1.94	1.75	1.85	**10.25**	OK
p,m-Xylene	2.01	2.13	1.83	2.38	1.91	2.01	1.80	1.91	**9.77**	OK
Pentachloroethane	0.32	0.33	0.25	0.25	0.24	0.29	0.23	0.21	**7.52**	OK
Pentadecane	2.19	2.63	1.89	2.65	1.97	2.47	2.18	2.15	**15.69**	OK
PGME	0.79	0.74	0.59	0.80	1.24	1.36	1.28	1.46	**12.36**	OK
PGMEA	1.46	1.42	1.10	1.61	1.93	1.97	1.87	2.22	**14.47**	OK
p-isopropyltoluene	-	-	-	-	-	-	-	-	**-**	-
Propylbenzene	1.99	2.05	1.99	2.02	1.88	2.05	1.96	1.98	**3.41**	OK
sec-Butylbenzene	1.99	2.07	1.98	2.04	1.88	2.10	1.97	1.99	**4.38**	OK
Styrene	1.74	1.84	1.50	2.05	1.58	1.62	1.53	1.62	**11.49**	OK
TAME	1.93	1.83	2.00	1.55	1.75	1.92	2.01	2.02	**9.76**	OK
tert-Butanol	1.02	0.91	1.18	0.87	1.19	0.98	1.21	1.21	**13.39**	OK
tert-Butylbenzene	1.97	2.04	1.97	2.01	1.86	2.08	1.95	1.98	**4.10**	OK
tert-Butyltoluene	2.15	2.36	1.96	2.67	2.03	2.27	1.95	2.05	**12.14**	OK
Tetrachloroethene	3.31	3.45	3.16	3.82	3.24	3.46	3.15	3.41	**7.75**	OK
Tetrachloromethane	2.12	2.02	1.90	1.95	1.85	2.01	1.93	2.00	**3.74**	OK
Tetradecane	2.43	2.84	1.99	3.16	2.25	2.64	2.45	2.65	**18.15**	OK
THF (tetrahydrofuran)	1.89	1.92	1.87	1.77	1.75	6.67	1.88	1.92	**41.35**	NOK
THT (tetrahydrothiofeen)	1.30	1.37	1.08	1.36	1.32	1.34	1.26	1.27	**8.23**	OK
Toluene	2.03	2.11	1.86	2.25	1.86	1.94	1.81	1.93	**7.43**	OK
trans-1,2-Dichloroethene	1.85	1.79	1.96	1.50	1.81	1.82	2.00	2.03	**9.45**	OK
trans-1,3-Dichloropropene	2.02	1.99	1.80	2.11	1.81	1.84	1.78	1.85	**5.87**	OK
trans-2-Methylcyclohexanol	0.86	0.78	0.55	0.95	1.31	1.30	1.21	1.63	**21.58**	NOK
trans-4-Methylcyclohexanol	0.31	0.34	0.19	0.49	1.03	0.95	0.83	1.29	**34.34**	NOK
trans-Decalin	2.33	2.59	2.15	2.88	2.17	2.40	2.09	2.17	**11.51**	OK
Tribromomethane	1.95	2.03	1.69	2.31	1.88	1.96	1.82	1.86	**11.24**	OK
Trichloroethene	2.21	2.19	2.10	2.33	2.14	2.24	2.28	2.32	**4.05**	OK
Trichloromethane	1.83	1.83	1.86	1.63	1.69	1.82	1.86	1.87	**5.45**	OK
Trichloromonofluoromethane	1.83	2.21	1.95	1.96	1.48	1.48	1.50	1.76	**8.80**	OK
Tridecane	2.04	2.37	1.76	2.53	1.82	2.12	1.84	2.00	**14.98**	OK
Undecane	2.03	2.34	1.83	2.53	1.85	2.07	1.80	1.88	**13.14**	OK
Vinylchloride	1.62	1.59	1.15	0.85	1.11	1.46	1.58	1.75	**14.74**	OK

Table 16. Raw data on the reproducibility with n=8, measured on the level of 10 mg/L, on GC-MS system 1.

Compound	1	2	3	4	5	6	7	8	Variation coefficient %	OK/NOK
1,1,1,2-Tetrachloroethane	9.69	8.59	11.88	9.86	8.26	10.52	9.57	7.73	**13.77**	OK
1,1,1-Trichloroethane	9.02	7.74	11.62	9.23	7.68	9.90	9.06	7.42	**14.96**	OK
1,1,2,2-Tetrachloroethane	6.75	6.24	8.51	6.73	5.45	7.13	6.47	5.10	**15.29**	OK
1,1,2-Trichloro-1,2,2-trifluoroethane	7.51	4.70	8.52	4.86	5.23	6.18	4.95	4.93	**25.94**	NOK
1,1,2-Trichloroethane	7.97	7.39	10.94	9.26	7.15	9.52	8.87	6.96	**14.68**	OK
1,1-Dichloroethane	8.02	6.39	9.90	7.16	6.65	8.06	7.43	6.11	**16.92**	OK
1,1-Dichloroethene	9.03	6.54	10.33	7.02	7.63	8.42	7.67	6.36	**19.12**	OK
1,1-Dichloropropane	8.69	7.81	11.49	9.38	7.58	9.81	9.30	7.52	**14.26**	OK
1,1-Dichloropropene	9.32	8.22	12.24	9.71	8.09	10.44	9.63	7.81	**14.85**	OK
1,2,3,4-Tetrahydronaphthalene	9.38	9.19	14.81	12.60	8.90	14.04	12.89	9.06	**20.86**	NOK
1,2,3-Trichlorobenzene	5.12	4.86	7.53	6.82	4.84	7.76	6.95	4.91	**20.75**	NOK
1,2,3-Trichloropropane	7.94	7.61	11.83	10.15	7.47	10.31	9.59	7.19	**16.17**	OK
1,2,3-Trimethylbenzene	8.78	8.20	12.30	9.97	7.97	10.85	9.99	7.57	**16.54**	OK
1,2,4-Trichlorobenzene	5.82	5.54	8.82	7.81	5.59	8.75	7.91	5.67	**19.99**	OK
1,2,4-Trimethylbenzene	9.26	8.48	12.79	10.43	8.36	11.30	10.40	7.88	**16.39**	OK
1,2-Dibromo-3-chloropropane	8.23	7.56	10.39	9.03	7.16	10.26	9.19	6.95	**17.00**	OK
1,2-Dibromoethane	9.18	8.13	11.44	9.49	7.73	10.03	9.11	7.49	**13.91**	OK
1,2-Dichlorobenzene	7.04	6.81	10.86	9.38	6.88	9.95	9.08	6.61	**17.86**	OK
1,2-Dichloroethane	7.66	7.01	9.97	7.88	6.53	8.48	7.86	6.48	**14.47**	OK
1,2-Dichloropropane	8.81	7.82	11.43	9.53	7.55	9.96	9.42	7.48	**14.81**	OK
1,2-Diethylbenzene	8.61	8.35	13.63	11.40	8.17	12.02	11.22	8.05	**18.94**	OK
1,3,5-Trichlorobenzene	6.91	6.56	10.63	9.16	6.66	10.09	9.19	6.57	**19.43**	OK
1,3,5-Trimethylbenzene	9.53	8.86	13.10	10.72	8.59	11.49	10.64	8.07	**15.96**	OK
1,3-Butadiene	7.73	5.25	9.56	6.97	4.32	7.44	6.77	6.55	**25.62**	NOK
1,3-Dichlorobenzene	7.63	7.27	11.75	10.01	7.34	10.50	9.61	7.03	**17.69**	OK
1,3-Dichloropropane	8.32	7.73	11.80	9.35	7.01	9.45	9.14	7.11	**16.17**	OK
1,3-Diethylbenzene	8.76	8.70	14.17	11.71	8.34	12.64	11.60	8.32	**19.78**	OK
1,3-Diisopropylbenzene	6.86	7.12	10.52	9.23	5.84	11.84	10.00	7.18	**27.08**	NOK
1,4-Dichlorobenzene	7.46	7.07	11.43	9.75	7.20	10.28	9.42	6.87	**17.67**	OK
1,4-Diethylbenzene	8.81	8.61	14.10	11.67	8.30	12.51	11.57	8.28	**19.71**	OK
1,4-Diisopropylbenzene	9.13	8.94	14.81	12.28	8.59	13.74	12.54	8.74	**21.67**	NOK
1,4-Dioxane	10.61	9.46	13.42	11.58	9.00	11.85	11.08	8.72	**14.44**	OK
1-Bromo-3-chloropropane	16.04	15.42	23.17	19.87	14.74	20.25	18.95	14.35	**15.85**	OK
1-Butanol	4.93	4.35	5.31	4.98	4.50	5.35	5.24	3.81	**13.68**	OK
1-Methyl-2-pyrrolidone	-	-	-	-	-	-	-	-	**-**	-
1-Pentanol	5.86	5.26	6.54	6.26	4.57	6.29	5.86	4.15	**16.99**	OK
2,2-Dichloropropane	10.14	8.12	10.90	8.14	7.83	8.87	8.25	6.85	**15.14**	OK
2,2-Dimethylbutane	8.38	5.95	11.17	6.35	5.94	7.34	6.20	5.86	**24.12**	NOK
2,3-Dichloropropene	9.64	8.44	11.22	8.98	8.01	9.69	9.15	7.54	**13.19**	OK
2,4-Dimethyl-3-pentanone	9.39	8.85	13.01	10.83	8.26	11.34	10.69	8.08	**16.30**	OK
2,4-Dimethylpentane	8.72	7.43	11.51	8.62	7.23	9.22	8.47	6.90	**16.14**	OK
2-Butanol	5.74	4.67	6.04	5.05	4.23	4.71	4.64	3.38	**15.20**	OK
2-Butoxy ethyl acetate	10.91	10.43	14.93	12.86	8.50	14.93	13.05	8.66	**24.71**	NOK
2-Chloro-1,3-butadiene	9.43	8.09	12.18	9.03	8.13	9.63	9.33	7.24	**15.97**	OK
2-Chlorotoluene	8.89	8.07	11.90	9.78	7.99	10.49	9.61	7.37	**15.45**	OK
2-Ethoxyethanol	5.09	5.74	6.21	6.81	3.81	6.07	4.87	3.71	**19.51**	OK
2-Ethoxyethyl acetate	12.00	10.87	15.87	13.28	8.91	13.96	12.22	8.87	**20.55**	NOK
2-Ethyltoluene	9.41	8.62	12.93	10.53	8.47	11.24	10.51	7.95	**16.00**	OK
2-Methoxyethanol	10.05	9.14	11.68	9.81	7.84	10.34	9.54	6.84	**16.72**	OK
2-Methyl-1-propanol	4.89	4.10	4.95	4.65	3.60	4.13	4.11	2.99	**13.85**	OK
2-Methyl-2-butanol	7.15	6.41	8.09	7.04	5.64	6.89	6.73	4.97	**14.21**	OK
2-Methylbutane	4.02	3.23	6.30	4.41	1.94	4.04	3.07	4.04	**30.45**	NOK
2-Methylcyclohexanone	10.57	10.22	16.70	24.22	16.98	21.98	20.93	13.16	**22.64**	NOK
2-Methylpentane	9.29	5.54	11.33	6.75	6.02	7.30	6.59	6.10	**26.38**	NOK
2-Pentanol	6.25	5.83	7.26	6.39	4.85	6.27	5.99	4.57	**14.07**	OK
2-Propoxyethanol	6.84	7.15	7.96	7.37	4.95	8.35	6.72	5.01	**21.01**	NOK
3-Chloro-1-propene (allylchloride)	-	-	-	-	-	-	-	-	**-**	-
3-Ethyltoluene	9.76	9.00	13.14	10.87	8.68	11.51	10.55	8.22	**15.11**	OK
3-Heptanone	9.36	9.07	14.12	12.88	9.16	13.15	12.16	8.91	**17.06**	OK
3-methyl-1-Butanol	5.54	5.02	6.33	5.62	4.22	5.63	5.39	3.94	**15.89**	OK
3-Methyl-2-butanone	9.62	8.62	12.44	11.63	10.56	12.88	12.07	8.68	**14.27**	OK
3-Methylcyclohexanone	9.69	9.38	14.89	-	52.29	53.45	49.22	15.68	**58.73**	NOK
3-Pentanol	6.63	6.00	7.62	6.79	5.29	6.73	6.42	4.88	**13.92**	OK
3-Pentanone	9.13	8.56	12.31	11.01	9.52	12.43	11.61	8.67	**14.62**	OK
4-Chlorotoluene	8.92	8.07	12.10	10.00	8.06	10.57	9.84	7.51	**15.45**	OK
4-Ethyltoluene	9.71	8.93	13.33	10.88	8.70	11.55	10.76	8.19	**15.85**	OK
4-Heptanone	9.37	9.16	13.98	12.14	8.99	12.60	11.81	8.62	**16.94**	OK
4-Hydroxy-4-methyl-2-pentanone	-	5.25	7.21	7.00	3.94	6.85	5.76	4.27	**41.53**	NOK
4-Methylcyclohexanone	9.53	9.36	14.59	-	41.38	-	-	14.81	**86.61**	NOK
4-Vinyl-1-cyclohexene	9.59	9.20	13.86	11.67	8.82	12.35	11.42	8.71	**16.38**	OK
5-methyl-3-heptanone	9.27	9.14	14.48	11.96	8.42	12.63	11.87	8.51	**19.53**	OK
Acetone	9.58	6.28	10.04	6.61	10.97	8.05	8.09	5.64	**26.56**	NOK
Allyl alcohol	3.27	2.19	2.49	2.45	2.14	2.01	2.06	1.78	**15.06**	OK
a-Methylstyrene	9.46	9.30	14.58	12.10	8.42	12.96	12.02	8.58	**20.21**	NOK
a-Pinene	9.21	8.87	14.27	11.93	8.44	12.40	11.18	8.45	**17.88**	OK

(Table 16 continuing)

Compound	1	2	3	4	5	6	7	8	Variation coefficient %	OK/NOK
Benzene	6.50	6.31	7.74	9.88	8.11	10.34	9.55	7.67	**14.42**	OK
Benzyl acetate	9.82	9.13	13.26	12.01	7.99	14.66	12.68	8.47	**25.52**	NOK
Benzyl alcohol	3.18	3.53	3.41	4.38	2.21	4.69	3.66	2.52	**30.20**	NOK
Benzyl chloride	11.92	11.33	17.08	15.68	11.10	16.54	14.28	10.34	**18.28**	OK
Bromobenzene	8.83	8.10	11.90	9.89	8.00	10.41	9.65	7.65	**14.32**	OK
Bromochloromethane	6.91	5.85	8.40	6.70	5.76	7.54	6.81	5.57	**15.42**	OK
Bromodichloromethane	8.27	7.39	9.73	8.00	6.93	8.52	8.00	6.64	**12.64**	OK
Bromomethane	3.10	2.04	2.98	2.19	1.35	2.75	1.98	2.11	**30.18**	NOK
Butyl glycidil ether	10.17	10.53	15.04	13.35	9.38	14.07	12.77	9.07	**19.05**	OK
Butylacrylate	10.39	10.01	14.81	12.12	8.39	12.43	11.49	8.59	**18.56**	OK
Butylbenzene	9.53	8.90	13.38	10.81	8.57	11.71	10.91	8.23	**16.74**	OK
Butylmethacrylate	10.94	10.40	16.49	13.15	9.25	14.55	12.61	9.16	**20.98**	NOK
Butylpropionate	10.63	9.72	14.87	12.77	9.22	13.15	12.40	8.99	**17.91**	OK
Chloroethane	4.52	2.80	4.42	3.43	2.12	4.60	3.35	3.89	**32.67**	NOK
Chloromethane	2.93	1.51	4.58	1.67	1.38	3.28	2.25	3.52	**51.64**	NOK
cis-1,2-Dichloroethene	7.88	6.74	10.05	7.59	6.70	8.32	7.85	6.15	**16.10**	OK
cis-1,3-Dichloropropene	8.39	7.77	10.94	9.42	7.29	9.71	8.98	7.16	**14.15**	OK
cis-2-Methylcyclohexanol	7.68	7.47	9.99	9.47	6.54	10.52	9.44	6.25	**21.95**	NOK
cis-4-Methylcyclohexanol	6.35	6.39	8.36	7.50	5.21	10.05	7.64	5.05	**26.91**	NOK
cis-Decalin	9.59	9.39	15.57	12.85	9.06	13.81	12.65	9.10	**19.87**	OK
Cumene	8.86	8.59	13.55	11.60	8.35	11.99	10.92	8.18	**17.15**	OK
Cyclohexane	8.26	7.12	11.09	8.59	6.63	9.36	8.25	7.18	**16.66**	OK
Cyclohexanol	6.31	5.98	7.33	7.39	5.12	7.64	6.96	5.00	**18.25**	OK
Cyclohexanone	9.37	9.22	14.39	-	54.68	57.59	56.14	15.79	**61.39**	NOK
Cyclohexene	7.92	9.35	10.45	7.73	6.39	8.60	7.84	8.29	**16.10**	OK
Cyclopentane	7.91	4.26	8.23	5.38	4.31	6.20	4.96	5.32	**28.94**	NOK
Cyclopentanone	9.12	8.34	13.00	20.26	18.55	22.99	20.24	11.49	**26.19**	NOK
Dibromochloromethane	8.54	7.82	10.27	8.81	7.37	9.33	8.67	7.03	**12.76**	OK
Dibromomethane	7.68	6.78	8.99	7.48	6.44	8.22	7.61	6.29	**13.43**	OK
Dibutyl ether	9.10	8.75	13.55	11.40	8.29	11.80	10.88	8.08	**17.35**	OK
Dichlorodifluoromethane	0.81	0.52	1.94	0.42	0.37	1.34	0.61	0.00	**94.22**	NOK
Dichloroethyl ether	11.76	11.43	17.78	15.63	11.19	16.25	14.89	10.92	**17.60**	OK
Dichloromethane	7.37	4.48	7.06	4.95	5.46	5.98	5.68	4.46	**23.12**	NOK
Diethylene glycol diethyl ether	9.66	9.14	13.84	12.28	7.46	15.42	12.30	7.90	**29.37**	NOK
Diisobutyl ketone	9.03	9.22	14.49	11.92	8.44	12.81	11.71	8.33	**20.05**	NOK
Diisopropylether	10.37	8.44	13.02	9.79	8.64	10.42	9.93	7.86	**16.24**	OK
Dimethyl formamide	-	-	-	-	-	-	-	-	**-**	-
Dipropylene glycol methyl ether										
D-Limonene	9.71	9.65	15.84	12.47	8.70	13.65	12.59	9.01	**21.29**	NOK
Dodecane	8.63	8.36	14.20	11.35	7.62	12.88	11.47	8.19	**23.09**	NOK
EPI	10.29	9.26	13.06	10.86	8.36	10.95	10.35	8.20	**14.58**	OK
ETBE	10.01	8.51	13.09	9.99	8.48	10.53	9.95	7.83	**15.89**	OK
Ethanol	2.92	2.04	1.67	1.71	2.47	1.63	1.86	1.18	**24.98**	NOK
Ethyl acetate	10.47	8.67	13.35	9.54	8.52	10.17	10.06	7.09	**19.28**	OK
Ethyl propionate	10.35	9.12	13.36	11.08	8.72	11.62	11.18	8.53	**15.96**	OK
Ethylacrylate	11.01	10.04	14.41	11.79	9.45	12.32	11.82	9.17	**15.08**	OK
Ethylbenzene	8.90	8.61	13.16	11.40	8.39	11.60	10.78	8.18	**15.82**	OK
Ethylene chlorohydrin	2.99	1.42	7.21	2.38	1.90	1.65	2.14	1.36	**46.55**	NOK
Ethylene glycol diethyl ether	9.69	9.38	13.75	11.78	8.55	12.18	11.29	8.49	**16.85**	OK
Ethylene glycol dimethyl ether	9.04	7.99	9.91	8.89	7.02	9.30	8.58	6.18	**16.25**	OK
Ethylene glycol methylether acetaat	12.29	11.01	14.98	13.19	9.15	13.38	11.95	9.08	**17.48**	OK
Ethylene glycol monobutyl ether	-	-	-	13.10	6.70	15.28	10.71	-	**80.75**	NOK
Ethylene glycoldiacetaat	11.86	11.88	15.02	12.62	8.50	14.40	12.63	8.48	**23.72**	NOK
Ethylether	9.66	6.77	11.02	7.42	8.12	8.51	7.72	6.22	**20.14**	NOK
Ethylmethacrylate	10.48	9.24	12.50	10.17	8.59	11.21	10.35	8.26	**14.95**	OK
Furfural	7.54	7.40	10.27	11.39	7.90	12.45	9.63	7.17	**19.26**	OK
Furfuryl alcohol	5.98	5.70	5.17	7.33	3.94	6.25	5.30	2.56	**31.83**	NOK
Hexachlorobutadiene	8.37	7.81	11.76	9.70	7.81	10.80	10.05	7.43	**17.11**	OK
Hexachloroethaane	8.57	7.78	12.26	9.86	7.83	10.38	9.65	7.39	**16.05**	OK
Hexadecane	6.88	6.72	10.76	8.87	5.36	12.21	9.99	6.73	**31.59**	NOK
Iodomethane	5.43	3.91	4.52	4.02	3.84	4.62	4.02	3.33	**15.37**	OK
Isobutyl acetate	10.47	9.51	13.81	11.81	8.96	12.41	11.55	8.93	**15.95**	OK
Isobutyl benzene	9.47	9.14	14.77	12.38	8.95	12.88	11.96	8.73	**18.02**	OK
Isophorone	7.12	7.19	10.38	9.41	5.98	11.84	9.73	6.79	**26.67**	NOK
Isooctane	-	-	-	-	-	-	-	-	**-**	-
Isopentyl acetate	10.63	9.62	14.83	12.54	9.30	13.17	12.22	8.98	**17.67**	OK
Isopropyl acetate	10.21	9.10	13.49	10.74	8.64	11.24	10.37	8.02	**15.75**	OK
Isopropyl glycidil ether	10.60	10.02	14.67	12.55	9.02	13.06	11.72	8.68	**17.67**	OK
Isopropyl glycol	7.20	6.77	8.28	8.09	4.88	8.14	6.38	4.78	**20.51**	NOK
MEK (2-Butanone)	10.02	8.16	12.46	15.07	16.81	17.35	16.60	10.74	**18.09**	OK
Mesityl oxide	-	-	-	-	-	-	-	-	**-**	-
Methacrylonitrile	8.77	7.34	11.05	8.25	7.62	8.82	8.52	6.37	**16.57**	OK
Methyl acrylate	11.47	9.62	14.50	10.84	9.77	11.47	11.29	8.35	**16.94**	OK
Methyl amyl ketone	9.88	9.93	15.74	17.08	11.88	15.49	14.55	10.74	**14.45**	OK
Methyl isoamyl ketone	9.92	9.65	15.12	16.85	11.83	15.83	14.67	10.40	**16.30**	OK
Methyl isobutyl carbinol	7.19	6.45	8.31	7.31	5.66	7.45	7.05	5.23	**15.46**	OK
Methyl isobutyl ketone	9.41	8.85	12.70	10.57	8.18	11.06	10.53	7.94	**16.02**	OK

(Table 16 continuing)

Compound	1	2	3	4	5	6	7	8	Variation coefficient %	OK/NOK
Methyl propyl ketone	9.80	8.95	12.74	12.87	11.47	14.20	13.83	9.45	**15.62**	OK
Methylal	-	-	-	-	-	-	-	-	-	-
Methylcyclohexane	-	-	-	-	-	-	-	-	-	-
Methylcyclopentane	8.29	6.81	10.80	8.20	6.63	9.03	7.92	6.96	**16.74**	OK
Methylmethacrylate	10.63	9.26	12.29	9.59	8.57	10.42	9.81	7.75	**14.69**	OK
Methyl-n-butyl ketone	10.50	10.13	15.12	16.34	12.26	15.73	14.81	10.92	**14.16**	OK
Monochlorobenzene	8.31	7.87	12.07	10.35	7.80	10.49	9.85	7.55	**15.10**	OK
MTBE	10.37	7.72	12.70	8.88	8.31	9.56	8.99	7.07	**18.96**	OK
n,n-Dimethylacetamide	-	-	-	-	-	-	-	-	-	-
Naphthalene	3.31	2.73	3.92	3.55	2.85	4.04	3.52	2.67	**17.38**	OK
n-Amyl acetate	10.82	10.17	15.62	12.98	9.15	13.31	12.46	9.22	**18.20**	OK
n-Butylacetate	10.33	9.70	14.03	11.80	8.46	11.81	10.92	8.32	**16.44**	OK
n-Decane	10.05	9.51	14.31	11.68	8.96	12.54	11.32	8.54	**17.08**	OK
n-Heptane	10.81	9.27	12.74	10.11	8.92	10.97	10.10	8.67	**13.32**	OK
n-Hexane	10.20	8.07	13.60	9.25	8.14	10.18	9.20	6.30	**22.08**	NOK
n-Nonane	10.43	9.45	13.93	11.26	8.98	11.74	10.81	8.67	**14.73**	OK
n-Octane	10.41	9.32	13.32	10.65	8.96	11.31	10.50	8.64	**13.84**	OK
n-Pentane	4.62	3.97	4.23	3.56	5.09	3.76	3.89	3.59	**13.70**	OK
n-Propanol	4.20	3.25	3.70	3.42	2.88	2.98	3.17	2.07	**17.61**	OK
n-Propyl acetate	10.53	9.38	13.67	11.20	8.97	11.77	11.22	8.59	**15.67**	OK
o-Xylene	8.41	8.08	12.63	10.87	7.96	11.11	10.31	7.71	**16.46**	OK
p,m-Xylene	8.80	8.43	13.05	11.20	8.30	11.54	10.67	8.02	**16.27**	OK
Pentachloroethane	0.32	0.21	0.39	0.20	0.14	0.24	0.16	0.14	**33.80**	NOK
Pentadecane	7.48	7.39	11.64	9.38	6.03	13.02	11.03	6.76	**31.92**	NOK
PGME	6.40	6.27	7.53	6.88	4.79	6.49	5.63	4.15	**15.50**	OK
PGMEA	12.54	11.31	15.66	13.27	9.63	13.79	12.60	9.36	**17.71**	OK
p-isopropyltoluene	-	-	-	-	-	-	-	-	-	-
Propylbenzene	9.68	8.95	13.19	10.77	8.69	11.39	10.69	8.15	**15.50**	OK
sec-Butylbenzene	9.70	9.00	13.38	10.92	8.68	11.64	10.85	8.21	**16.13**	OK
Styrene	7.73	7.58	11.40	9.80	7.12	10.39	9.54	7.01	**17.91**	OK
TAME	10.52	9.03	12.20	9.60	8.50	10.35	9.71	8.09	**13.77**	OK
tert-Butanol	6.57	4.30	6.45	4.61	4.92	4.43	4.41	3.18	**22.39**	NOK
tert-Butylbenzene	9.55	8.83	13.28	10.78	8.64	11.47	10.67	8.10	**15.95**	OK
tert-Butyltoluene	9.14	8.94	14.85	12.29	8.68	13.16	12.04	8.62	**19.80**	OK
Tetrachloroethene	15.94	15.09	22.47	19.54	15.12	20.43	18.89	14.60	**14.88**	OK
Tetrachloromethane	9.23	8.13	11.64	9.62	7.77	10.42	9.34	7.66	**14.82**	OK
Tetradecane	7.97	8.03	13.14	11.39	6.88	14.01	12.30	8.38	**28.07**	NOK
THF (tetrahydrofuran)	8.29	7.30	10.68	8.50	7.13	16.76	8.23	6.74	**30.77**	NOK
THT (tetrahydrothiofeen)	6.11	5.24	8.14	6.25	5.90	8.89	7.69	5.83	**20.37**	NOK
Toluene	8.98	8.41	12.44	10.86	8.25	11.12	10.31	8.11	**14.49**	OK
trans-1,2-Dichloroethene	9.58	7.09	11.57	8.21	7.73	8.89	8.44	6.73	**18.54**	OK
trans-1,3-Dichloropropene	8.25	7.59	10.89	9.49	7.18	9.63	8.95	7.04	**14.51**	OK
trans-2-Methylcyclohexanol	6.70	6.91	8.87	8.40	5.85	9.31	8.20	5.72	**20.58**	NOK
trans-4-Methylcyclohexanol	5.17	5.33	6.37	6.41	4.24	7.94	5.88	4.45	**23.63**	NOK
trans-Decalin	9.82	9.65	15.73	13.15	9.31	13.84	12.76	9.29	**18.88**	OK
Tribromomethane	7.72	7.73	11.30	10.00	7.36	10.54	9.58	7.15	**16.80**	OK
Trichloroethene	9.89	9.15	13.32	11.56	9.39	12.05	11.59	9.18	**13.31**	OK
Trichloromethane	7.36	6.37	9.55	7.27	6.35	7.96	7.46	5.86	**15.92**	OK
Trichloromonofluoromethane	5.77	4.50	8.21	6.23	3.01	6.02	4.69	5.10	**27.06**	NOK
Tridecane	8.06	8.05	13.30	10.73	7.15	12.72	11.45	8.06	**24.54**	NOK
Undecane	8.44	8.38	13.65	11.36	7.97	12.00	11.12	8.00	**19.48**	OK
Vinylchloride	3.75	2.07	3.11	2.23	1.78	4.03	3.13	4.29	**37.62**	NOK