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Identification of Sources for Illegal Oil Spills by Using GC-MS (Gas Chromatography and Mass-Spectrometry) Databases and Multivariate Statistics

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Environmental Toxicology and Chemistry
Submission date: November 2011
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Partial fulfillment of the requirements for the Degree of Master of Science in Environmental Toxicology and Chemistry

at

Department of Chemistry
Faculty of Natural Sciences and Technology

NTNU – Trondheim
Norwegian University of
Science and Technology

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November 2011

ABSTRACT

Preparing a defensible oil spill fingerprinting is always challenging. Presently available well established method for this purpose is a univariate method by comparison of diagnostic ratio using repeatability limit as suggested by European Committee for Standardization (CEN)-method. The consistency result of this method, however, tends to depend on the skill of the analyst who performs the analysis. The shortcoming of CEN-method was then demonstrated by the application of the method to the "MS Server" and "MV Full City" oil spill cases. The author's analysis result exposed some discrepancies when was compared with the one performed by SINTEF. Therefore, this thesis focuses on the effort of pursuing alternative or at least complimentary methods to ease the shortcoming of the CEN-method. The main investigation was then emphasized on the possibility of employing the multivariate analyses, i.e. principal component analysis (PCA), cluster analysis, and partial least square discriminant analysis (PLS-DA). The performance of those multivariate analyses were examined by applying to the case studies of "MS Server" and "MV Full City" oil spills. Later on, it was found that PCA failed to classify the samples properly according to the match or non-match with the reference samples. The power of the PCA was revealed when the method was combined with the cluster analysis. The PCA combined with the cluster analysis demonstrated to be faster and undoubtedly more objective (in term of the analyst skill and expertise) as compared to the CEN-method. PLS-DA also showed the same benefits. Moreover, the PLS-DA gives more similar result to the CEN-method applied by SINTEF (irrespective of the difference gaps of the analysts skill, i.e. the SINTEF researchers v.s. the author) as compared to the PCA combined with the cluster analysis. However, the main drawback of the PLS-DA is the requirement of quite large number of sample to obtain a good result. At last, we could see that there is possibility of applying several multivariate analyses, i.e PCA combined with the cluster analysis, and PLS-DA, for the alternatives or complementary of a well established univariate analysis of oil spill fingerprinting (CEN-method). In order to develop the alternative method(s) properly, further research is needed, especially the one which employs more controllable samples.

ACKNOWLEDGMENTS

It has been a great honor for the author to be supervised by Professor Bjørn K. Alsberg who were very patiently guided the author through the complexity of chemometrics and scientific writing. The author also would like to express her gratitude to Dr. Per J. Brandvik, who act as co-supervisor, for invaluable discussion and guidance in the field of oil spill fingerprinting. The author acknowledges SINTEF for providing necessary oil spill data and reports. The support from Department of Chemistry, Faculty of Natural Science and Technology, NTNU, by providing license for the multivariate statistical software *The Unscrambler* is also acknowledged. Special thanks goes to Thea Berg Finnes who helped the author to take care of administrative issue during the thesis.

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ACRONYMS

PCA principal component analysis

PLS-DA partial least square discriminant analysis

CEN European Committee for Standardization

ROV remote operating vehicle

GC-FID gas chromatography and flame ionization detection

GC-MS gas chromatography and mass spectrometry

DR diagnostic ratio

PAH poly-aromatic hydrocarbon

QA quality assurance

RSD relative standard deviation

PLS partial least square

DP diagnostic power

RMSEP Root Mean Square Error of Prediction

1

INTRODUCTION

1.1 BACKGROUND AND MOTIVATION

Marine oil spill is a kind of pollution, which is characterized by releasing oil into the ocean or coastal waters from tankers, offshore platforms, drilling rigs, oil wells, marine pipelines, etc. Oil spill early detection is necessary and it's fingerprinting is needed to indicate the spill source for early action and also needed for defensible prosecution. In the first place, oil spill fingerprinting could be seen as *threatening* to the owners and/or operators. However, it should be considered as preventive and repressive environmental protection as well as beneficial tool for responsible industrial and shipping practice. For the case of marine pipeline, oil spill fingerprinting allows early identification of the leaking pipeline and gives clue about which pipelines are suspected to be leaked prior to confirmation by remote operating vehicle (ROV) inspection, which is a very expensive operation. In this case, oil spill fingerprinting proved as a highly cost effective tool for early action to cope with oil spill [Sinclair and Grigson, 1996]. Another case of the usefulness of oil spill fingerprinting is for the purpose of defensible prosecution. Along with other tools, i.e. automatic identification (navigation/positional) systems fitted on vessels, the oil spill fingerprinting (or DNA tagging, as usually called) offer precise identification of the pollution culprit [Al-Khudhairy, 2002].

All crude oils and petroleum products have chemical compositions that differ from each other. This variability in chemical compositions results in unique chemical "fingerprints" for each oil and provides a basis for identifying the source of the spilled oil [Wang et al., 1999]. However, when oil spilled into the sea, it is subjected to variety of weathering processes, such as spreading, evaporation, dispersion, dissolution, oxidation, emulsification, and bio-degradation. It is obvious that as soon as the oil spills, it spreads over the water surface. Lighter oil components dissolves into sea water or evaporate to the air. Hydrocarbons can react with oxygen (oxidation), which may either lead to the formation of soluble products or persistent tars. In moderate to rough seas, most spilled oils will take up water droplets and form water-in-oil emulsions under the turbulent action of waves on the sea surface. Bio-degradation is also take place because sea water contains a range of marine micro-organisms capable of metabolizing oil compounds. All of these processes change the chemical and physical composition of the spilled oil [ITOPF, 2002].

Having the changing of the spilled oil composition taken into main consideration, the basic idea of oil spill identification (fingerprinting) is to identify a set of components present in most oil types, which changes as little as possible due to weathering processes, such that we are able to give convincing and defensible evidence about the origin of the spilled oil. The relative composition of these components (two, three, and four ring structures) reflects the biogenic input, source, migration and reservoir conditions of the oil. These components are called as bio-markers.

Ratios of selected bio-markers are used to identify the source of an illegal oil spill by systematic profile comparison between the oil spill and one or several possible sources [Al-Khudhairy, 2006]. One of the method is called the European Committee for Standardization (CEN)-method for oil spill identification and it is well established method. It is now applied as an international standard and is based on using univariate statistics. In order to be valid to state that there is a match between the oil spill and the possible source, only 2 out of total 27 bio-marker ratios can be significantly different.

Even though CEN-method for oil spill identification is a standardized method, application of this method relies on the skill of the analyst. This is because crude oils and petroleum products are complex mixtures of chemical compounds, thus it is not feasible to identify and quantify all individual compounds in the mixture [Christensen and Tomasi, 2007].

The fact that the established method uses univariate statistics, makes it interesting to discover whether multivariate statistics can be alternatives as well as complementary methods. An example of earlier work for this purpose was done by Christensen and Tomasi [2007]. They summarized several studies using principal component analysis (PCA) for oil hydrocarbon fingerprinting and also established integrated multivariate oil fingerprinting method that are rapid, objective and comprehensive. Their general steps on approaching this problem was adopted in this thesis.

1.2 PROBLEM DESCRIPTION

The main issue in this thesis is to define and characterize alternative statistical method(s), preferably among the multivariate analysis, on the oil spill fingerprinting. Detail of the problems are as follow.

1. Demonstrate the well-established univariate analysis based on CEN method on the oil spill fingerprinting and give comments about it's robustness, benefits, and drawbacks.

2. Demonstrate the application of three available multivariate statistical methods, i.e. PCA, hierarchical cluster analysis, and partial least square discriminant analysis (PLS-DA), to solve the same oil spill fingerprinting problem in point 1 and give comments about it's robustness, benefits, and drawbacks.

3. Compare the performance among multivariate statistical methods as well as with the univariate one.

1.3 OBJECTIVES

The main focus on this thesis is to propose alternative statistical method(s), preferably among the multivariate ones, which could perform better or at least similar with the univariate method. It is also expected that the proposed multivariate alternative could overcome the drawback of the univariate method and act as an additional tool.

1.4 RESEARCH METHODOLOGY AND WRITING SCHEME

In order to solve the problems in Sect.1.2 and to achieve the objectives in Sect.1.3, a research methodology was designed and executed. The results were reported according to the following writing scheme:

1. In order to fuel the author with the knowledge of the oil spill fingerprinting as well as the available multivariate statistical analyzes, the state of the art of these topics were summarized in Chapter 2.

2. The bulk of the data utilized in this thesis were the gas chromatography and flame ionization detection (GC-FID) chromatogram, gas chromatography and mass spectrometry (GC-MS) response, and diagnostic ratio (DR) of bio-markers and poly-aromatic hydrocarbon (PAH)s for two oil spill cases, i.e. "MS Server" and "MV Full City". The reports of the oil spill fingerprinting (in Norwegian) for those two cases [Faksness et al., 2010; Almås et al., 2007] were also available and the summary, including samples description, is given in Chapter 3. Moreover, Chapter 3 also contains spatial description of the samples, which describes relatives distance between samples and the wrecked ship.

3. Even though the two cases above have been thoroughly analyzed by SINTEF researchers by means of CEN-method, for the sake of demonstration of the corresponding method (see Sect.1.2), the author repeated the analysis according to author's limited knowledge on the CEN-method as well as the oil spill fingerprinting case. Based on these demonstrations, some comments about it's robustness, benefits, and drawbacks, especially related to the analyst who performing the CEN-method, were given. This is reported in Chapter 4.

4. Three multivariate analyzes were selected to be applied in this oil spill fingerprinting, i.e. PCA, hierarchical cluster analysis, and PLS-DA. Those three methods were implemented to the two cases of "MS Server" and "MV Full City" and the results are reported in Chapter 5, 6, and 7 respectively.

5. The results from the univariate analysis and multivariate analyzes were then tabulated and compared. Comments about their performance were also given. This is reported in Chapter 8.

6. Chapter 9 concludes the work and gives suggestion about the alternative multivariate method that possibly is able to overcome the drawback of the univariate method and acts as an additional tool. Suggested future works are also given in the same chapter.

2 OIL SPILL, IT'S UNIVARIATE FINGERPRINTING AND ALTERNATIVE MULTIVARIATE ANALYZES

In this chapter, the author talks about some terms which are related to oil spill investigation. First, the composition and properties of crude oil are reviewed. Subsequently, the description about weathering processes, which are important when oil spill accident occurred, are described. The univariate oil spill fingerprinting is represented by CEN-method and briefly explained. Finally, three alternative multivariate analyzes (PCA, cluster analysis, and PLS-DA) are summarized to conclude this chapter.

2.1 CRUDE OIL COMPOSITION AND PROPERTIES

Crude oil is a name for organic compounds, which is in a liquid form under reservoir condition. Crude oil is a mixture of hydrocarbon compounds in varying proportion. The organic compounds that composing crude oil can be divided as pure hydrocarbon and heteroatomic organic compounds. Some of them also contain sulfur, oxygen, phosphorus, and nitrogen. They also contain minor constituents such as porphyrins, ash-forming metal compounds (usually sulfides of vanadium, nickel, copper, cobalt, molybdenum, lead, chromium, and arsenic), inorganic salts, hydrogen sulfide, and water in varying amounts. The average carbon contents in the crude oil is of ca. $79.5 - 88.5 wt\%$, hydrogen contents of ca. $10 - 15.5 wt\%$, and impurity contents of up to a maximum of 5 wt % [Barker et al., 2007].

2.1.1 *Hydrocarbon*

Hydrocarbon is the major compound in crude oil. It is divided into two classes, i.e saturated and unsaturated or aromatic hydrocarbon. The saturate hydrocarbon includes normal alkane (or paraffin), branched alkane (or isoparaffin), and cycloalkane (or naphthene). Number of carbon atom in the saturated hydrocarbon that compose crude oil varies. An important sub groups of paraffin is wax. This compound contains more than 20 carbon atoms. Commonly, the world's crude oil contents of $2 - 15\%$ wax. Aromatic hydrocarbon composing a crude oil also varies from benzene to polyaromatic hydrocarbon, such as phenantrene, benzopyrene etc.

2.1.2 *Heteroatomic Organic Compounds*

Heteroatomic organic compounds are a group of organic compounds that contains not only hydrogen and carbon atoms but also small amount of oxygen, nitrogen, sulphur and some trace metal. Two of most important groups in these compounds are resins and asphaltenes.

Resins are relatively polar compared to hydrocarbons. They often have surface-active properties. Their molecular weights ranging from $700 - 1000$. They contain functional group like carboxylic acid, phenol and sulphoxides.

Asphaltenes are large molecules with molecular weight $1000 - 10000$. They consist of polyaromatic compounds with $6 - 20$ aromatic rings and side chains. They can be classified as *hard* and *soft* asphalts. Crude oil can contain up to 6%wt *hard* and 10% wt *soft* asphaltene [Al-Khudhairy, 2006] .

2.1.3 *Crude oil Properties*

Physical properties of crude oil vary. This is because of variation in composition of organic compounds content. Therefore, it's physical properties such as density, odor, boiling point, viscosity, etc have been used to classify oils.

- Boiling point. Boiling point of crude oil usually can be used to classify the lightness of crude oil. Light crude oils usually contain greater number of hydrocarbon with low boiling point, and paraffinic hydrocarbons, while heavy crude oils contain greater amounts of hydrocarbon with high boiling point and asphalt-like molecules [Barker et al., 2007]. More over, boiling point can be used the weathering process of the oil when it spill to the water column. Oil with high boiling point tend to evaporate faster then oil with low boiling point. This will also give benefit to oil spill spill investigation.

- Viscosity. Viscosity of liquid is defined its resistance to flow. In oil spill related problem, the unit that usually used is centipoise (cP). Total viscosity of the oil depends on the viscosity of its constituent components. Crude oil which contain lower molecular weight components will have lower viscosity compared to crude oil which contain higher molecular weight components.

- Density. Density of crude oil are vary from 0.78to0.99kg/L at 150° C. Crude oil, which contains greater amount of lower molecular weight component has lower density as compared to crude oil that has a greater amount of higher molecular weight component.

- Pour point. Pour point is a temperature at which oil is unable to flow when subjected to a slight movement, when it is cooled without disturbance under specified laboratory condition. It can also be defined as a temperature when an oil become solidify. Oil containing a greater amount of wax will have a higher pour point.

- Flash point. Flash point is a temperature when the oil start to generate gas or vapor generated by heating an oil starts to be ignited by a flame. Oil contains greater number of lower molecular weight compounds will have lower flash point [Al-Khudhairy, 2006].

2.2 WEATHERING OF OIL SPILL

When oil is spilled into water, it immediately undergoes various chemical, physical, and biological processes. Those processes are called weathering. The weathering processes change the chemical and physical properties of the oil. Thus, it affects the oil spill investigation. The degree of spilled oil weathering process depends on the original chemical and physical properties of the spilled oil, environmental condition when the oil spilled, and the properties of the water. Fig.2.1 shows schematically the weathering process in the water.

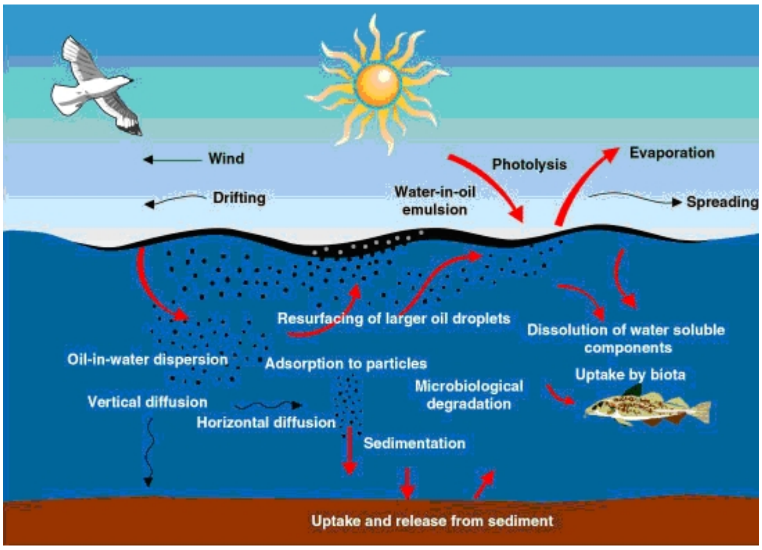

Figure 2.1: Weathering process of oil spill in the sea.

2.2.1 *Evaporation*

Evaporation occurs soon after the oil is released to the water column. Evaporation rate is affected mostly by vapor pressure of the component in the spilled oil. Usually, lighter components in the spilled oil (compounds with number of carbon atoms up to 12) or compounds with boiling point lower than 200°C evaporates within 24 hour period after spilled. Other factors that affect the evaporation rate are wind speed, thickness of the spilled oil, mousse formation and water/air temperature. Evaporation affects the oil spill fingerprinting. Lighter crude oil which contains lighter component will be more difficult to fingerprint because it may evaporate within a few hours. While, heavy crude oil, which contains compounds with higher molecular weight, tends to evaporate slightly, thus will be easier to be fingerprinted [Stout and Wang, 2007].

2.2.2 *Dissolution*

Dissolution of oil component into water occurs simultaneously with evaporation. Usually the most soluble compounds in the spilled oil are also the most volatile one. Studies have shown that evaporation dominates the losses of spilled oil. Therefore, evaporation effect to oil spill fingerprint is more significant compare to dissolution [Stout and Wang, 2007].

2.2.3 *Emulsification*

Crude oil contains surface-active compounds that can make it form a water/oil-emulsion if the energy at the sea surface is sufficient. Formation of water/oil emulsion is the only weathering process that makes crude oil persistent on the water surface. Emulsion can inhibit another weathering processes such as dissolution, evaporation, photo oxidation and bio degradation of hydrocarbon [Stout and Wang, 2007].

2.2.4 *Bio-degradation*

Sea water contains many kinds of microorganisms. When oil is spilled into water column, some of these microorganisms use oil components as an energy source. Almost all types of oil components can be degraded by microorganisms. The easiest oil components to be degraded are the straight chain saturated hydrocarbons with number of carbon atoms 10 to 22. The most difficult oil components to be degraded by microorganisms are cycloalkanes, resins, and asphaltenes. Biodegradation of spilled oil occurs slower than evaporation or dissolution. It's effect on an oil spill fingerprinting is also not clear in the short term after release. Compounds that are biodegraded commonly are converted into their oxidized states. These compounds can be further degraded, dissolved, or retained within the oil. Chemical fingerprinting tends to focus on the compounds that are unable to degrade or are less degradable. These compounds are called petroleum biomarker and PAH [Stout and Wang, 2007].

2.2.5 *Photo-oxidation*

Under the influence of sunlight, spilled oil in the water can undergo several reactions that produce some oxygen-containing compounds such as peroxides, aldehydes, ketones, sulfoxides, epoxides and fatty acids. These derivative compounds are usually more soluble as compared to the parent compounds. Thus, they can be removed from the environment. However, hydrocarbon with higher molecular weight can form cross-links upon photo-oxidation. Thus, the derivative compounds become more insoluble as compared to the parent compounds. The rate of photo-oxidation of crude oil depends on the intensity of ultraviolet radiation on sunlight [Stout and Wang, 2007].

2.3 OIL SPILL IDENTIFICATION USING CEN-METHOD

The following description of CEN-method was taken from Al-Khudhairy [2006]. CEN-method for oil spill identification is a method issued by European Committee for Standardization to identify whether an oil spill is related to the source or not. This method consists of two parts. The first part (Part 1) is about sampling techniques and handling of the oil samples prior to their arrival at a laboratory, which will carry out the analysis. The second part (Part 2) covers general concepts and laboratory procedures of oil spill investigation methodology, including analytical techniques, data treatment, data processing and interpretation/evaluation of the result. Since this thesis focuses on the data analysis, only the latter part (Part 2) will be briefly discussed in this section.

The main technique to be used to identify oil spill is to compare the spills with the suspected sources. The comparison is performed by evaluating the chromatographic patterns, i.e GC-FID and GC-MS, of the spills and the sources. A spill sample could be considered as identical to the suspected source if one of the following requirements is fulfilled.

1. No significance different in GC-FID and GC-MS chromatograms, or

2. any observed differences are from changes introduced when collecting samples after a spill, e.g because of weathering, contamination, mixing, etc.

Otherwise, the sample could be concluded as not identical to the suspected source.

CEN-method for oil spill identification introduces diagnostic ratio to the basic technique of oil spill identification. Diagnostic ratio is a ratio between the peak height or peak area of single compound or compound group selected by their diversity in chemical composition in petroleum and petroleum products and on their known behavior in weathering processes. The diagnostic ratio is generated from GC-MS data of selected PAHs and biomarkers compound that are robust against weathering and the diversity in chemical composition of oils from different wells and oil types. In order to reduce the variance, ratios are generated by using the area or peak height of compounds, which are recorded by the same m/z value and that are within the same reasonable retention time range.

In the CEN-method, the decision chart for oil spill identification consist of three level as shown in Fig.2.2. The first level (Level 1) is GC-FID screening analysis of all spilled samples and suspected samples. Data from this screening should be used for the following purposes.

1. Characterizing of the oil sample(s) by obtaining the overall boiling (carbon) range of the oils, i.e. the total distribution of hydrocarbons including n-alkanes from C10 to C40, if present.

2. Visual inspections of the chromatograms for possible characteristic features and a tentative classification to a type of the spilled oil.

3. Establishing selected acyclic iso-prenoid ratios readily determined using GC-FID.

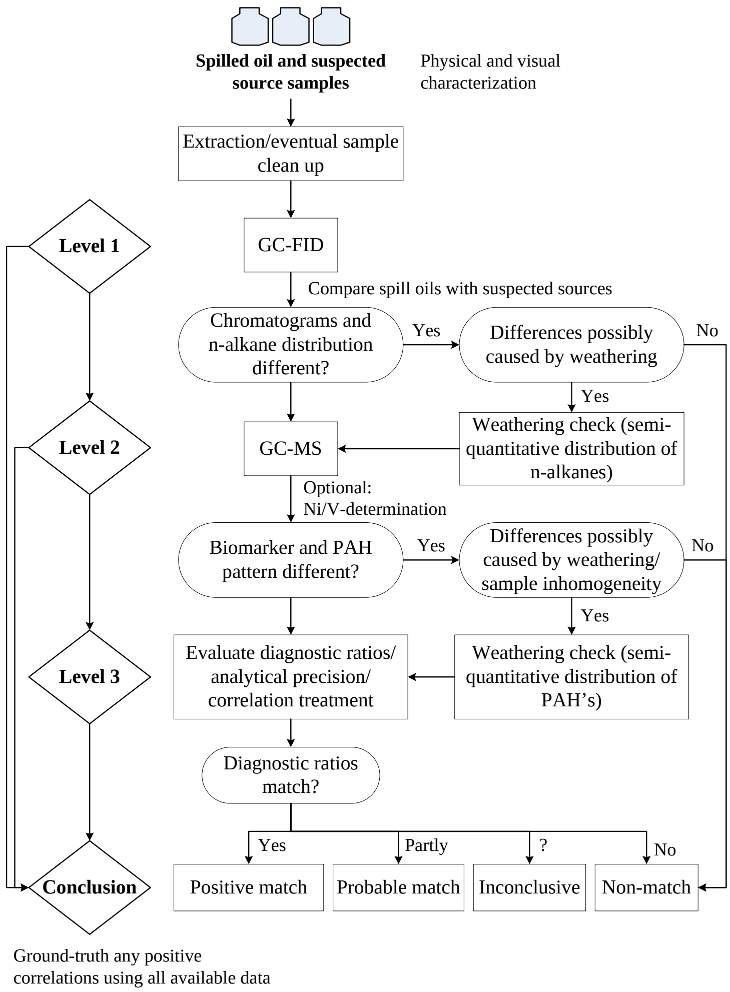

Figure 2.2: Decision chart for oil spill identification [Al-Khudhairy, 2002].

If the chromatograms of spilled sample and suspected sources are different and the differences are possibly from weathering, the next level (Level 2) should be performed. If the differences are not caused by weathering, the sample must be eliminated for the next level analysis or concluded as non match to the suspected sources.

The second level (Level 2) is GC-MS fingerprinting. In this level, the samples are analyzed using gas chromatography combined with mass spectrometry in the selected ion monitoring mode (GC-MS-SIM). Data from this level of analysis should be used for the following purposes.

1. Visual inspection of the ion profiles in the chromatograms for possible characteristic features, and an oil type classification of the spilled oil.

2. In order to generate diagnostic ratios based on an evaluation of the presence and "robustness" of the diagnostic PAHs and biomarkers.

If the pattern of biomarker and PAHs of the spilled samples are different from the suspected sources, and the differences are possibly due to weathering, the sample should be performed a weathering check. After weathering check, if the pattern differences due to weathering, then the sample should continue to the next level. But if the differences are not due to weathering, the sample should be concluded as non match.

Data obtained in this level should be used to generate diagnostic ratios of selected biomarkers and PAHs. Before integrating the compounds applied for calculating the diagnostic ratios, a visual inspection of the diagnostic ion chromatograms should be carried out to eliminate some of the recommended diagnostic peaks that may not be present in sufficient concentrations. This step is useful in order to establish robust diagnostic ratios. Also, a visual comparison of the ion chromatograms is advised to enable exclusion of obviously different samples.

The PAHs used for oil spill identification are the dibenzothiophenes and the phenanthrenes. In addition, the C1-pyrenes/fluoranthenes/benzofluorenes are included. In total there are ten recommended diagnostic ratios to be used, that are derived from PAHs. The biomarkers selected for the analysis are terpanes, steranes and mono- and tri-aromatic steranes. These biomarkers are commonly to be used within organic geochemistry and oil spill identification. These biomarkers are useful because of their specificity, diversity and resistance to biodegradation and weathering. For the purpose of identification of the oil spill source, at least 19 suites of biomarker's diagnostic ratio are available. Another group of biomarker that can be used for identification of oil is Sesquiterpanes, therefore it may be included as an optional group of biomarkers. Sesquiterpanes are a group of bicyclic (C14-C16 polymethyl-substituted decalins) biomarkers that comprise one of the largest terpenoid classes. In GC-MS chromatograms these compounds may be examined by their characteristic fragment ions (m/z123, 179, 193 and 207). There are four recommended diagnostic ratios that can be used for oil spill identification. Sesquiterpanes are low boiling compounds, so they are easily evaporate. Therefore, the use of sesquiterpanes diagnostic ratio for oil spill identification is an optional. Only valid if the samples are not weathered.

The next level (Level 3) is evaluation of the data. At this level, the results obtained from level 1 and 2 should be used for the following purposes.

1. Assessing the impact of weathering based on a weathering check of n-alkane data from level 1 and the semi-quantitative distribution of the PAH groups from level 2. The weathering checks are performed optionally.

2. Deciding which diagnostic ratio can be used for comparison based on oil type and analytical variance, and which samples should be reanalyzed because of heterogeneity.

3. Comparison of diagnostic ratios data using repeatability limit.

4. Visual comparison of generated ion chromatograms to check the results of the ratio comparison (ground truth all data).

In this method, to estimate an acceptable difference between two samples, repeatability (r) is applied. Repeatability is a test method to compare individual ratios, assuming that the two samples to be compared are originating from the same source. Repeatability conditions are met when the samples are analyzed in one series. If the repeatability limit is exceeded, it is beyond reasonable doubt that this assumption is not valid and that the samples are originating from different sources. The protocol/decision chart for diagnostic ratio evaluation can be seen in Fig.2.2.

The repeatability limit of validation is based on standard normal distribution. Determining the repeatability standard deviation, S_r, of an analysis method depends on the quality assurance (QA) system of the laboratory. In general, it is calculated by analyzing samples relevant for a method at least seven times in one series when a method is taken into use and if the method has to be validated. Calculation of the standard deviation or relative standard deviation (RSD) reveals r. CEN-method for oil spill identification, choose a fixed repeatability RSD of 5% for S_r . The RSD = 5% limit can be seen as a quality criterion.

The repeatability limit $r_{95\%}$ is calculated by multiplying the fixed RSD (S_r) with a factor 2.8 as follows.

$$r_{95\%} = 2.8 \times 5\% = 14\% \tag{2.1}$$

This means when the samples are analyzed under repeatability conditions, each ratio with an S_r of 5% may not differ more than 14%. The critical difference (CD) is calculated as follows.

$$CD = \frac{mean \times r_{95\%}}{100} \tag{2.2}$$

When the value of the critical difference (CD) based on the repeatability limit for one of the ratios between two samples is higher than the absolute difference measured, the samples are accepted as a positive match.

The results from all analytical levels should be specified either as a Positive Match, Probable Match, Inconclusive or Non-Match. A Positive Match means the spill and the source samples are identical beyond reasonable doubt. Both GC-MS and GC-FID chromatograms show no differences or the differences are caused by weathering. The diagnostic ratio evaluation also show that the differences are below repeatability limit. A Non-Match means a condition when the chromatograms of the spilled and the source samples are different and the differences can not be explained by weathering and the several diagnostic ratios are outside the repeatability limit. If only very small differences are observed, or if only just one pair of ratios is outside the repeatability limit, a Probable Match can be concluded for the samples. If the total amount of oil in the samples are very low, and analytical variance of the diagnostic peaks is high, the differences of diagnostic ratios may be higher than repeatability limit. This would imply the elimination of so many diagnostic ratios from further comparison so that it can be concluded as Inconclusive [Al-Khudhairy, 2002].

2.4 MULTIVARIATE ANALYSIS OF OIL SPILL IDENTIFICATION

2.4.1 *General*

Multivariate analysis has been used for hydrocarbon fingerprinting since the beginning of 1980s, but the application of oil hydrocarbon fingerprinting in environmental forensic is relatively recent, i.e in the middle of 1995s. Common methods to be used for this oil hydrocarbon fingerprinting are PCA and factor analysis such as performed by Aboul Kassim in 1995 and Simoneit in 1995, Burns et al in 1997, Lavine et al in 2001, Stout et al 2001 etc [Christensen and Tomasi, 2007]. Other method such as cluster analysis is also known to be used such as performed by Sun et al. [2009] and partial least square (PLS) as performed by Mudge [2002]. Four steps of multivariate analysis for oil spill identification includes chemical analysis, data pre-processing, numerical analysis and statistical test [Christensen and Tomasi, 2007]. Flow chart of the method is presented in Fig.2.3.

In this master thesis, sample preparation and chemical analysis step was excluded. Therefore, the description is solely for the other 3 subsequently steps. Since the analyses performed in this work were utilized DR, the second step, i.e. data pre-processing, the description focuses on the selection of DR.

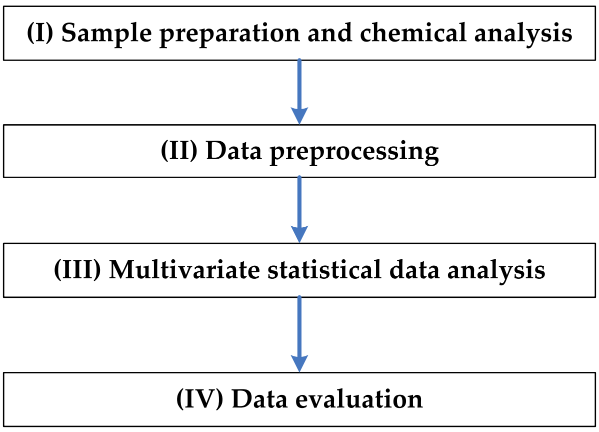

Figure 2.3: Flowchart of Multivariate Method for Oil Spill Fingerprinting. Adopted from [Christensen and Tomasi, 2007].

2.4.2 *Pre-processing of Diagnostic Ratio Data*

Diagnostic ratio (DR) is a ratio between the peak height or peak area of single compounds or group of compounds selected for their diversity in the chemical composition in petroleum and petroleum product and their reported response to weathering processes [Hansen et al., 2007]. DR has been widely used in geochemistry for oil correlation, determination of organic input and precursor, depositional environment, assessment of thermal maturity, and evaluation of in-reservoir oil biodegradation [Wang et al., 2007]. The application of diagnostic ratios in oil spill fingerprinting was based on this geochemistry literature. The benefit of using diagnostic ratio for oil spill finger printing are [Wang et al., 2007]:

1. Diagnostic ratios can minimize concentration effect.
2. Diagnostic ratios have self normalized effect so that it can reduced any variations due to instrumental operating condition.

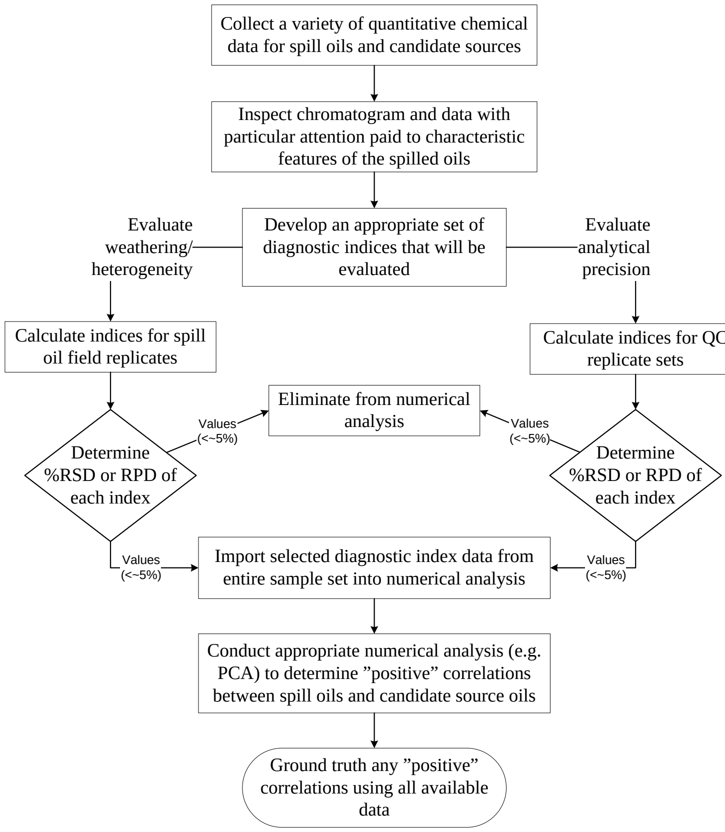

Figure 2.4: Flowchart for evaluation of diagnostic ratio of oil spill fingerprinting [Stout et al., 2001].

Nevertheless, not all diagnostic ratios can be used for the analysis. Only source ratios or ratios of compounds that are robust to weathering processes can be used for oil spill fingerprinting. Selection of appropriate ratios should be based on oil type, weathering condition and the distribution of target compounds [Yang et al., 2008]. Diagnostic ratios selection is also important in order to keep uncertainties to a minimum level, such that the result will be more reliable. Otherwise, improper ratio selection will result an incorrect correlation result [Yang et al., 2008].

There are many methods to select the diagnostic ratios to be used for the analysis in order to generate reliable result. Christensen and Tomasi [2007] used diagnostic power (DP) to select diagnostic ratio. DP is defined as the relative standard deviation of a diagnostic ratio in oils with different origin (RSD_V) divided by relative standard deviation of a diagnostic ratio of samples (RSD_A). CEN methodology select diagnostic ratio using signal to noise (S/N) test. This method only uses peaks with $S/N > 3$ to 5 for comparing diagnostic ratio [Al-Khudhairy, 2006]. In this thesis, method suggested by Stout et al. [2001] which excluded ratios with relative standard deviation of triplicate sample (RSD_A) larger than 5% is adopted (See Fig.2.4).

2.4.3 *Principal Component Analysis*

PCA is an appropriate tool when we have a number of observed correlated variables and would like to develop a smaller number of latent variables (which are called principal components) that represent most of the variance in the observed variables. The principal components may then be used as criterion variables in subsequent analyses. For our purpose of oil spill fingerprinting, the variables thrown into PCA should be the diagnostic ratios. All oil spill samples, including the ones used as (candidate) references, are treated as the data set. The first and second principal components (or more) may be used as criterion variables. If we observe score plotting of these first two criterion variables, the clue to classify the oil spill sample may be obtained. Any samples clustering together with reference sample, shown in score plot, could be categorized as ”match”, while the ones away from reference samples (outliers) could be considered as "non match".

Mathematically, PCA is defined as an orthogonal linear transformation that transforms the data to a new coordinate system such that the greatest variance by any projection of the data comes to lie on the first axis (called the first principal component), the second greatest variance on the second axis, and so on [Jolliffe, 2002]. Technically, a principal component can be defined as a linear combination of optimally-weighted observed variables.

The PCA model can be written as

$$\mathbf{X} = \mathbf{T}\mathbf{P}^{\mathsf{T}} + \mathbf{E} \tag{2.3}$$

where $\mathbf{X}$, $\mathbf{T}$, $\mathbf{P}$, and $\mathbf{E}$ are the data matrix, the scores matrix, the transposed loadings matrix, and the residual matrix, respectively.

The size of data matrix $\mathbf{X}$ is $N \times K$. The N represents the number of object included in the analysis. For our case the object is the oil sample. While K represents the number of variable involved in the analysis. For our case, the variables are biomarkers and PAH. The data matrix $\mathbf{X}$ itself contains the diagnostic ratios.

The matrix operation in Eq.(2.3) can be well illustrated by the following diagram.

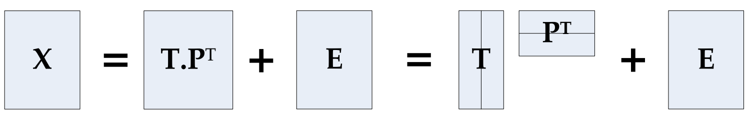

Figure 2.5: Illustration of PCA model.

The loading matrix contains the weights needed to define the direction of the latent variable axis in the original space. The loading weights p_j are the coefficients in the linear combination of the original variables:

$$t_i = p_1 x_1 + p_2 x_2 + \ldots + p_K x_K \tag{2.4}$$

where t_i is the score for object i for one principal component, p_j is the loading associated with variable x_j, and M is the number of original variables. It is noted that the scores are the coordinates of the object along the new latent variables.

2.4.4 *Hierarchical Cluster Analysis*

The term of cluster analysis refers to a a class of technique which has an objective to divide a set of samples or object into several groups or cluster. The main criteria of this divisions is that the clusters are homogeneous and samples in the same group are more similar to each other compare to samples in the other groups [Bratchell, 1992].

Hierarchical cluster analysis is one of the most popular clustering technique and widely used because of its simplicity, rapid to compute and gives straightforward and intuitive interpretaion. In this technique, objects which are most similar are merged into larger cluster [Bratchell, 1992]. This technique has been used in several studies for oil spill investigation. Sun et al. [2009] used cluster analysis for fingerprinting of oil spill in China Bohai sea using GC-FID and GC-MS data. Shigenaka and Jr. [1996] also used cluster analysis to asses bioavaibilty of PAH in several location three years after Exxon Valdez oil spill. This method meets the criterion for oil spill forensic that are fast, comprehensive, and unsupervised [Christensen and Tomasi, 2007].

Hierarchical cluster analysis are based on the measurement of distance or similarity between objects. Similarity between objects is satisfied by considering the spatial distances between points: objects with similar measurements are located close each other. Distance is governed by three conditions [Bratchell, 1992].

$$\begin{aligned} &\text{(i) } D_{ij} \geqslant 0;\ D_{ij} = 0 \text{ if } \mathbf{x}_i = \mathbf{x}_j \\ &\text{(ii) } D_{ij} = D_{ji} \\ &\text{(iii) } Ds_{ia} + D_{ja} \geqslant D_{ij} \end{aligned} \tag{2.5}$$

where D_{ij} denotes the distance between to objects i and j. Condition (i) and (ii) confirm that the measure is positive and symmetric. Symmetry means the distance from point i to point j is equal. Condition (iii) is called the metric inequality and distinguishes between metric distance and non-metric dissimilarities. This condition confirm that the direct distance between two points is less than or equal to that measure via a third point [Bratchell, 1992].

Measurement of a distance is based on several types of variable, i.e. categorical and continuous variable. Categorical variable is a variable that the values function as label rather than as number. This variable includes binary variable and ordinal variable [Sherrod, 2003]. Binary variable is variable which denote division into two categories. Usually the values of this variables are 0 and 1. The simplest similarity measurement of categorical variable is using matching coefficient in which for kth variable is given by [Bratchell, 1992].

$$\begin{aligned} s_{ijk} = &\ 1 \text{ if } x_{ik} = x_{jk} \\ s_{ijk} = &\ 0 \text{ if } x_{ik} \neq x_{jk} \end{aligned} \tag{2.6}$$

Another matching coefficient proposed by Jaccard, so called Jaccard coefficient, was given by [Bratchell, 1992].

$$\begin{aligned} s_{ijk} &= 1 \text{ if } x_{ik} = x_{jk} = 1 \\ \text{ignored if } x_{ik} &= x_{jk} = 0 \\ s_{ijk} &= 0 \text{ if } x_{ik} \neq x_{jk} \end{aligned} \tag{2.7}$$

Ordinal variable is categorical variable in which the category has logical order. The most appropriate distances for this variable are Manhattan or city-block distance. For $k-$th variable, the city-block distance is given by [Bratchell, 1992].

$$d_{ijk} = |x_{ik} - x_{jk}| \tag{2.8}$$

and the similarity measure is

$$s_{ijk} = 1 - d_{ijk} \tag{2.9}$$

Continuous variable is a variable which has numeric value (for chromatography peas, boiling point etc) [Sherrod, 2003]. For this variable, euclidean distance is the best known and the most appropriate distance [Bratchell, 1992]. The distance is given by

$$d_{ij}^2 = (x_i - x_j)(x_i - x_j)' \tag{2.10}$$

Instead of measuring distance or similarity between objects, hierarchical cluster analysis also considers the measurement of inter-cluster distance or distance between clusters. There are several types of inter-cluster distance. This thesis focuses on the three most common distances, i.e. the nearest neighbor distance, the average link distance, and the furthest neighbor distance.

The nearest neighbor, also called single linkage, uses the smallest distance between objects in two clusters [Bratchell, 1992].

$$d(r,s) = \min(\mathrm{dist}(x_{ri}, x_{sj})), i \in (i, ..., n_r) \tag{2.11}$$

The average linkage measures the distance between cluster centroids [Bratchell, 1992].

$$d(r,s) = ||\bar{x_r} - \bar{x_s}||_2 \tag{2.12}$$

where

$$\bar{x_r} = \frac{1}{n_r}\sum_{i=1}^{n_r} x_{ri}$$

While the furthest neighbor, also called complete linkage, measures the largest distance between clusters [Bratchell, 1992].

$$d(r,s) = \max(\mathrm{dist}(x_{ri} - x_{sj})),\ i \in (i, ..., n_r),\ j \in (i, ..., n_s) \tag{2.13}$$

The results of hierarchical cluster analysis is shown graphically by a dendrogram. Dendrogram is a tree-like structure which shows the series of merges between objects and clusters and the similarities at which they occur. Typical dendrogram is shown in Fig.2.6.

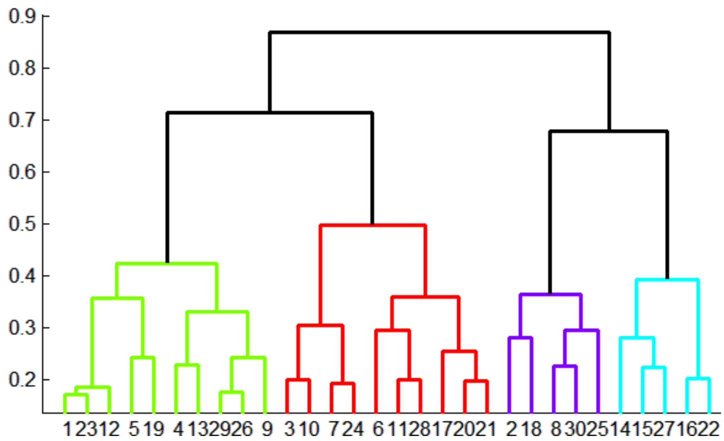

Figure 2.6: Example of a dendrogram.

2.4.5 *Partial Least Square - Discriminant Analysis (PLS-DA)*

PLS-DA is a supervised classification method based on PLS algorithm. As in any supervised classification method, the class information is stored in **Y** matrix. Here we have two datasets stored in **X** and **Y** matrix. **X** contain independent variables and information will be dependent to **Y**. This matrices are related through regression relationship. Process to find this relationship is called calibration step. This process is often called training step or learning step.The model gives reliable results and reliable predictive ability, if it has a low Root Mean Square Error of Prediction (RMSEP). RMSEP is a direct measurement of prediction error in **Y**. Once a model found by calibration step, it can be applied to new data. This is called as prediction step. In this step, the new **X**-data are projected onto principal or PLS components. **Y** was estimated using these projected scores and loading matrices. During prediction, uncertainty limit can be calculated from validation variances, the residual variances, and the leverage of **X**-data in the prediction objects. This uncertainty limit called deviation. Smaller deviation interval means the prediction sample is very similar to the training sample. The larger deviation interval means the new sample is more different from the training sample [Esbensen et al., 1994].

In oil spill case, once a model has been developed based on data (information about the references or source or suspect), it can be used to predict new data we want to know whether it is match to the references or not. Moreover, Barker and Rayens [2003] suggest that PLS, and not PCA, to be used for dimension reduction in connection with discrimination purposes when a training set is available.

PLS-DA gives qualify model, if all procedure is applied properly. Therefore, the data sets should be divided into training set, validation set and test set. The number of samples needed to accurately describe such classification problem increases exponentially with the number of variables measured [Westerhuis et al., 2008]. This will be a problem when the number of sample is small such that separation into training set, validation set and test set is not possible. In order to overcome this problem, cross validation is often used. In the cross validation, one or more samples are temporary taken out from the data set.

The rest of samples can be used in calibration step to predict error. This process is repeated until all samples in the data set is taken out. The cross validation makes better use of the data when separation into the three sets is not possible.

2.4.6 *Data Evaluation*

The fourth step of multivariate analysis for oil spill investigation is data evaluation. Several methods have been used to evaluate the output from multivariate analyses and to classify whether an oil spill is match or not to the suspected source.

In PCA, the most straightforward and intuitive method for data evaluation is through visual inspection of score and loading plots [Christensen and Tomasi, 2007]. A cluster can be distinguished based on their size, shape, or curved arrangement of the objects. More often, this classification is difficult because the objects form several clusters, which have different shapes and densities [Bratchell, 1992]. Therefore, the objectivity of matching process of spill and source oil samples can be improved by numerical comparisons and statistical tests. Christensen and Tomasi [2007] summarized several methods performed in many studies. Other numerical comparison using student's-t is also recommended by [Faksness et al., 2002]. These comparisons and statistical tests need replicated data such as score value or diagnostic ratios.

3 FULL CITY AND SERVER OIL SPILL CASE STUDIES: SAMPLE DESCRIPTION

3.1 COVERAGE

This chapter is intended to present the available and utilized data for this thesis, which was taken from two oil spill case studies, i.e. "MV Full City" and "MS Server". In fact, these cases were thoroughly investigated by SINTEF and related summary of the result is described here. Later on in Chapter 4-7, the univariate and multivariate analyzes upon both oil spill cases are presented and in Chapter 8 comparison between the SINTEF's result and the author's result is given. The SINTEF's result is the one which is presented in this chapter. This chapter also elaborates additional information, which is not covered by SINTEF's reports (i.e. Faksness et al. [2010] and Almås et al. [2007]), such as spacial consideration among the samples and relative distance between the suspected spill and the spill source (shipwreck location).

3.2 FULL CITY

MV Full City is a Panama flagged bulk cargo carrier. Her length is 167 meters. Because of bad weather, MV Full City grounded at 31st of July 2009 at 00:23 local time, close to the town of Langesund in Telemark, Norway. See Fig.3.1. At the time of grounded, MV Full City hauled approximately 1000 tons of heavy bunker oil (IFO 180) and 120 tons of marine diesel oil on board. Water penetrated into all cargo holds except cargo hold number #1 and all double-bottom tanks. The fore- and after-peak were not penetrated. Oil residues were observed in all cargo holds and in the engine room [Kystverket, 2009b].

Figure 3.1: MV Full City oil spill accident [Kystverket, 2009b].

The oil spill was present and observed from Larvik to Grimstad. It was also found oil lumps in several places down to Mandal. The oil lumps were suspected from MV Full City accident [Kystverket, 2009a]. For identification, SINTEF has received 58 samples under the auspices of the Norwegian Coastal

Administration (Kystverket). The samples were taken at the accident location and further south along the coast from the areas around Oddane to Mandal. In addition, SINTEF has also received 67 samples from Bamble Sheriff Office (both regional samples and reference oils from damaged ship), see Faksness et al. [2010]. Overview of the sample description is shown in Table 3.1.

Table 3.1: Sample description for oil spill fingerprinting of Full City accident [Faksness et al., 2010].

SINTEF ID	Location	Date	Description
2009-0472	Oddane, Vestfold	31-Jul	sand/stones contaminated with oil
2009-0473	Oddane, Vestfold	31-Jul	sand/stone not visible contamination
2009-0474	Oddane, Vestfold	31-Jul	thick oil washed up on beach
2009-0482	Krogshavn	2-Aug	teflon
2009-0483	Krogshavn	2-Aug	heavy oil and teflonpad
2009-0484	Krogshavn	2-Aug	litle oil sample with bark, etc
2009-0485	Krogshavn	31-Jul	20 liter with smooth, fine emulsion pumped up in Krogshavn
2009-0486	Landoy, Mandal	3-Aug	oil with traces of free water
2009-0487	Hanestangen, Kristiansand		water with black particles (pliers?), no oil smell (received 7 August)
2009-0489	Barge by unloading	6-Aug	sample 21, taken by E. Lydersen, saksnr. 108-27053
2009-0490	Såstein	7-Aug	sample 23, made by E. Lydersen, saksnr. 108-27053
2009-0491	Nevlunghavn, Ødegårdsfjord	6-Aug	1-15 mm thick, taken in Steinvik in Ødegårdsfjord, Nevlunghavn
2009-0492	Krogshavn	7-Aug	scraped off from the steep, solid rock, sample from deep pools in the mountains (5-10mm thicknesses)
2009-0493	Langesund Bad	7-Aug	langesund bad, 1 mm, Krogshavn.
2009-0494	Nevlunghavn, Ødegårdsfjord	6-Aug	emulsion foam absorbent booms to .....
2009-0495	Mølen	6-Aug	thick emulsion.
2009-0499	Hassletangen Grimstad	2-Aug	ruakerkilen outside the entrance, viscous coating spring stones.
2009-0500	Fie, Risør	1-Aug	petroleum lumps (about 5 mL)
2009-0501	Arendal komm.	7-Aug	oil with soil and sand
2009-0518	Barge 1	8-Aug	car no. 2
2009-0521	Barge 1	8-Aug	car no. 29
2009-0522	Barge 2	8-Aug	car no. 2
2009-0525	Barge 2	8-Aug	car no. 18
2009-0579	Såstein	6-Aug	oil from bay within havarist

Continued on Next Page...

SINTEF ID	Location	Date	Description
2009-0602	Cargo no 2	1-Aug	sample no 1 (oil from ”FullCity”)
2009-0603	Cargo no 3	1-Aug	sample no 2 (oil from "FullCity")
2009-0604	Cargo no 4	1-Aug	sample no 3 (oil from "FullCity")
2009-0605	Cargo no 5	1-Aug	sample no 4 (oil from "FullCity")
2009-0606	Machine room	1-Aug	sample no 5 (oil from "FullCity")
2009-0609	Vysotsk, Damanskiy	17-Jul	IF180 (sealing No. 9487431)
2009-0614	Skagen Roads	30-Jul	LS180 (sealing No. 0027014)
2009-0616	Skagen Roads	30-Jul	HS180 (sealing No. 0027074)
2009-0622	Lyngholm, Lillesand	19-Aug	
2009-0624	Napa, Vestfold	25-Aug	taken in trawl at 160 m depth
2009-0630	Barge 3	26-Aug	sample 3209-5
2009-0634	Barge 3	26-Aug	sample 3209-28
2009-0736	Krogshavn	19-Oct	petroleum lumps from HC Ramp
2009-0737	Krogshavn	19-Oct	mud from the sandy beach
2004-0355	Sample taken from ”Rockness”		
2004-0626	Sample taken from Åskoy in connection with "Rockness" accident		

The references to be used for the analysis should be the oil samples from the wrecked ship and probably also the samples from the location of accident as soon as possible after the accident happened. It means for this case, all samples from MV Full City tanks must be treated as reference samples. Another possibility for the reference sample is the oil sample obtained from the ship (and/or skimmer) that was used for collecting the oil spill.

However, referring to SINTEF report for ”MV Full City” oil spill, samples from Oddane (2009-0472), Såstein (2009-0579) and Krogshavn (2009-0485) are chosen as reference. Those samples are clearly from the surrounding area where the accident took place. The reason of the selection is because there were relatively large mark-up of oil in the area soon after the accident. While, samples from the tanks of MV Full City itself (SINTEF ID: 2009-0602, 2009-0603, 2009-0604, 2009-0605, and 2009-0606) were not selected as the reference. This is surprising for some extent. Why were the samples from the tanks of the wrecked ship disregard as reference? The author guesses that probably the sample from the MV Full City's tanks were in the intact condition, which means no weathering and no contamination at all affected the samples. It could be difficult to have the spill samples match with, especially for the ones which heavily weatherized and severely contaminated. Therefore, the samples, which more and less experienced weathering process but hundred percents sure that the samples were indeed from the Full City spill, were preferable to be selected as reference. By doing this, it was expected that the other spill samples do not differ very much with the reference.

The map of the samples location is shown in Fig.3.2. The map in Fig.3.2 was developed with the help of kart.finn.no based on tabulated data in Table 3.1. It shows sample locations along the east coast of Norway, stretched out from Larvik to Mandal. It is merely approximate locations in order to give overview about the relative distance between the sample and the accident location. The relative distance is tabulated in Table 3.2.

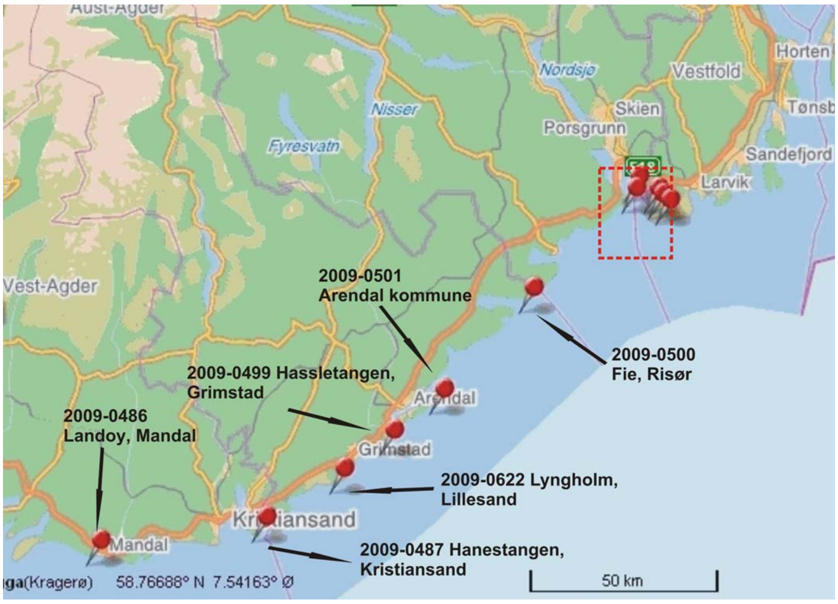

Figure 3.2: Approximate sample locations of Full City accident along the east coast of Norway, stretched out from Larvik on the North to Mandal on the South.

Table 3.2: Relative distance of the sample locations to the Full City shipwreck accident.

Locations	**SINTEF ID**	**Dist.(km)**
Cargo no 2	2009-0602	na
Cargo no 3	2009-0603	na
Cargo no 4	2009-0604	na
Cargo no 5	2009-0605	na
Machine room	2009-0606	na
Såstein	2009-0490	na
Krogshavn	2009-0482, 2009-0483, 2009-0484, 2009-0485, 2009-0492, 2009-0736, 2009-0737	3.3
Langesund Bad	2009-0493	3.7
Mølen	2009-0495	6
Oddane	2009-0472, 2009-0473, 2009-0474	7.7
Napa, Vestfold	2009-0624	9.5
Nevlunghavn, Ødegårdsfjord	2009-0491, 2009-0494	9.8
Fie, Risør	2009-0500	40

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Locations	SINTEF ID	Dist.(km)
Arendal kommune	2009-0501	75
Hassletangen, Grimstad	2009-0499	100
Lyngholm, Lillesand	2009-0622	115
Hanestangen, Kristiansand	2009-0487	145
Landoy, Mandal	2009-0486	190
Vysotsk, Damanskiy	2009-0609	na
Skagen Roads	2009-0614, 2009-0616	na
Barge 1	2009-0518, 2009-0521	na
Barge 2	2009-0522, 2009-0525	na
Barge 3	2009-0630, 2009-0634	na

The map in Fig.3.3 is a zoomed version map of the sample locations around the vicinity of the MV Full City shipwreck accident as shown as red dashed-line in Fig.3.2. The red dots represent coastlines where there is a registered mark of oil. The map was reproduced based on the one given in SeilMagasinet [2009] and then the sample data was added into it.

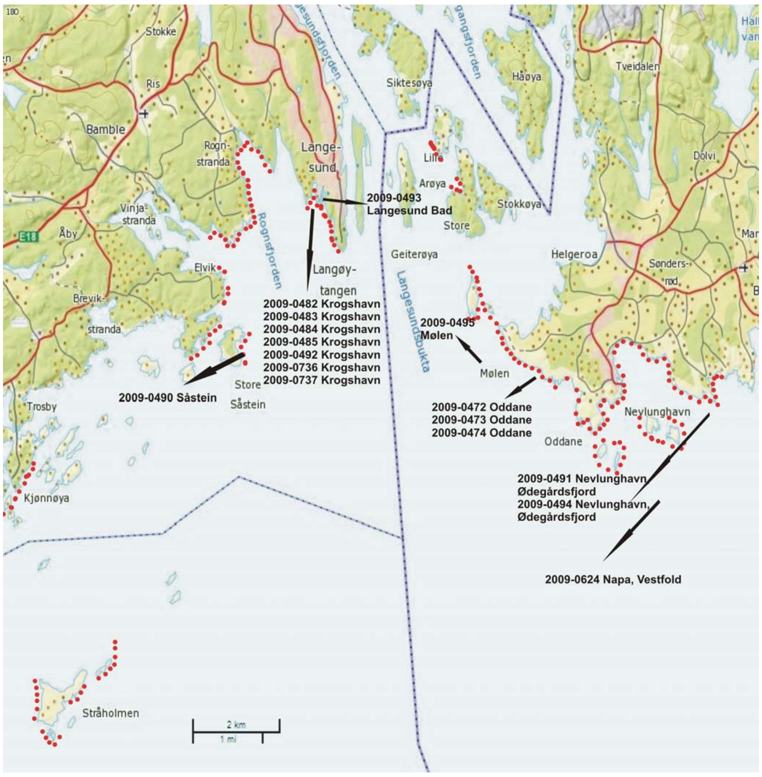

Figure 3.3: Sample locations of MV Full City accident in the close vicinity of the shipwreck scene.

Data received by the author were GC-FID chromatogram of the samples, the peak response of bio-marker and PAH compounds for each of the samples, and DRs generated from GC-MS response. The data was produced by SINTEF and the result of the corresponding fingerprinting was reported in Faksness et al. [2010].

3.3 SERVER

The Cyprus-registered cargo ship MS Server went on the ground next to Hellesøy lighthouse, just south of Fedje in Hordaland, at 18.30, Friday, 12 January 2007. The ship is owned by Cypriot Avena Shipping. It was southwest stiff wind ($15 - 16$ m/s) in the area when the grounding occurred, and wave height was about seven meters. It was announced that the ship was broken into two, see Fig.3.4. MS Server had 585 tons of heavy fuel oil and 72 tonnes of diesel on board when it grounded. The ship broke into two on the place of the largest oil tank was located. This tank contained 290 cubic heavy oil. It was likely that all of the contents have leaked out.

Figure 3.4: MS Server oil spill accident [Kystverket, 2007a,b,c,d]. She broke into two. The upper figures show the forepart of the ship, while the lower figures show the afterpart which sunk completely near Hellesøy lighthouse.

The influence area estimated were around 134 km far [Kystverket, 2007e]. Almås et al. [2007] developed a statistical map showing the probability of contamination due to MS Server oil spill accident. The map probably could be used as guidance on taking the samples. For oil spill fingerprinting purpose, SINTEF received 45 samples taken from the wreck of MS Server and the areas along the coast around Bergen and north of Gryllefjord of Troms. The samples were taken in the period of 13 January to 16 July. The samples consist of oil samples and birds feathers polluted by oil. SINTEF ID, sampling date and the description of the sample can be seen in Table 3.3.

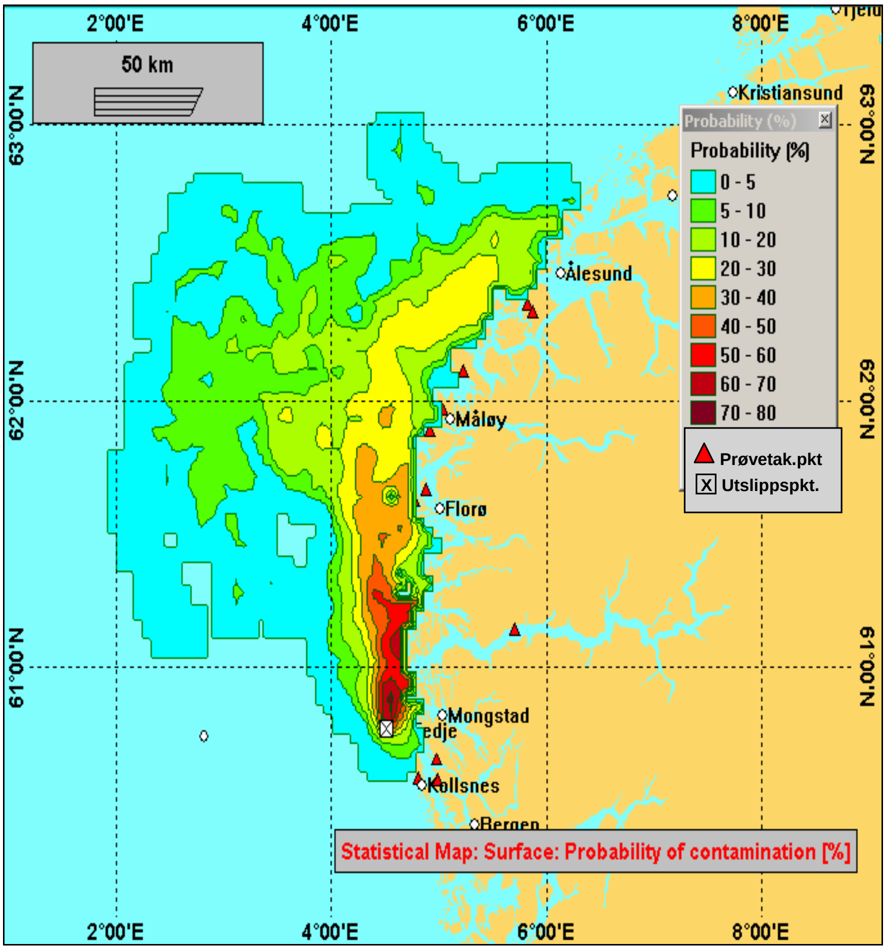

Figure 3.5: Probability of contamination due to MS Server oil spill accident [Almås et al., 2007].

Table 3.3: Sample description for oil spill fingerprinting of MS Server accident [Almås et al., 2007].

SINTEF ID	Date	Description/Location
2007-0010	14.01	Emulsion, taken up by the sea of KV Ålesund
2007-0011	14.01	Emulsion, taken up by the sea of KV Ålesund
2007-0012	13.01	Emulsion, from skimmer head to KV Eigun on deck
2007-0014	14.01	PadSample from sheet/rainbow Oil film outside the lihgthouse at Fedje
2007-0015	14.01	Emulsion scraped off the rocks at Innarøyene
2007-0016	14.01	Emulsion from scrapped the rock. Only patchvis Oil in the area around the scrapped
2007-0017	13.01	Emulsion from ”TV-bukta” by the lighthouse on Fedje. Sample from Sturla Dyregrov
2007-0018	14.01	Sample included Teflon pad, Herdla Vest

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SINTEF ID	Date	Description/Location
2007-0019	14.01	Kelp from rullestein strand, Herdla vest
2007-0020	14.01	Emulsion, from east of Sauøy (farm Øygarden)
2007-0021	14.01	Oil/Emulsion from lense, Gudbrandsøy
2007-0022	*	Oil from shipwreck - "Server": Sample from Tank 2
2007-0023	*	Oil from shipwreck - "Server": Sample from Tank 3
2007-0024	*	Oil from shipwreck - ”Server": Sample from Tank 4
2007-0025	18.01	Oil sample from sandy beach, Selje kommune
2007-0026	18.01	Oil sample (nr. 1), v/Kanneasteinen-Oppedal, Vågsøy kommune
2007-0027	18.01	Oil sample (nr. 2), Vågsøy kommune
2007-0028	16.01	Oil sample (nr. 1), Rognaldsvåg Havn, Fyllingskaien, Flora kommune
2007-0029	18.01	Oil sample (nr. 2), Båsund/Skorpa, Flora kommune
2007-0030	19.01	Oil sample (nr. 3), Båsund/Skorpa, Flora kommune
2007-0033	17.01	Oil sample collected at KV ”Eigun”
2007-0042	29.01	Oil sample, Osnessanden, Ulstein Kommune
2007-0055	23.01	Oil sample from pool, Fedje kommune
2007-0056	22.01	Oil sample (nr. 1), v/Gullbransøyna, Post 4
2007-0057	15.01	Oil sample, Radøy, Syltavågen
2007-0058	19.01	Oil sample, Radøy /Marøy/Leitevågen
2007-0059	31.01	Oil sample (nr. 4) MS Server, Gulen
2007-0060	31.01	Oil sample (nr. 13) MS Server , Gulen
2007-0061	31.01	Oil sample (nr. 18) MS Server, Gulen
2007-0062	28.01	Oil on birds (gulls)Onøy, Lurøy
2007-0063	2.02	Oil sample, Kvamsøy, Sande Kommune,
2007-0064	31.01	Oil sample, Stongholmsvikjo, Bømle kommune
2007-0065	31.01	Oil klatt, Ivasanden, Ulstein
2007-0066	31.01	Bird feathers from gannets (nr. 3), Ivasanden, Ulstein
2007-0067	31.01	Bird feathers from guillemot/razorbills (nr. 4), Ivasanden, Ulstein
2007-0068	31.01	Bird feathers from dead eiders (nr. 5), Osnessanden, Ulstein

Continued on Next Page...

SINTEF ID	Date	Description/Location
2007-0069	19.01	Sample from bucket of contaminated seawater, Hamsundpollen, Hamarøy kommune.
2007-0070	30.01	Bird feathers from wounded seagull (skårunge), Træna
2007-0084	31.01	Oil sample from kelp and grass, Okstadvika, Herøy
2007-0105	*	Oil sample from Eide, 9380 Gryllefjord
2007-0118	8.03	Oil sample (nr. 27 eller 22), Austrheim
2007-0119	8.03	Oil sample (nr. 27 eller 22), Austrheim
2007-0282	25.04	Oil sample, Vetvika, Bremanger kommune, Nordfjord
2007-0394	16.07	Oil sample (nr. 1), Fyrsundet position 2, Fedje
2007-0395	16.07	Oil sample (nr. 2), Fyrsundet position 2, Fedje

Again, the references to be used for the analysis should be the oil samples from the wrecked ship and probably also the samples around the area of accident as soon as possible after the accident happened. It means for this case, all samples from MS Server tanks must be treated as reference samples. The samples taken at Fedje at the day after accident should be treated as reference sample as well. Another possibility for the reference sample is the oil sample obtained from the ship (and/or skimmer) that was used for collecting the oil spill. Thus, it should be at least 8 reference samples, i.e oil from tank 2, tank 3, tank 4, and other tanks of MS Server (if exist, but no information is available for this), emulsion samples taken by KV Ålesund and KV Eigun and emulsion from TV-bukta near the lighthouse at Fedje.

SINTEF report for MS Server oil spill case uses only 4 oil samples as references, i.e sample from tank 3 and tank 4 of MS Server, sample taken by KV Eigun and sample from TV bukta near the lighthouse at Fedje. It is interesting to put forward a question why was tank 2 not being considered as reference. The reason was not mentioned. Sample from other tanks, for example tank 1 was not considered. Logically, if there is tank number 2, 3, and 4, there should be tank number 1. Or probably there is also tank number 5, 6, etc. However, there is no information about tank number 1 in the report, as well as other tanks. There was sample taken from KV Ålesund. It was not considered as reference sample. No reason is mentioned in the report. If KV Ålesund was involved during the oil spill cleaning operation, any sample taken should be considered as reference sample.

Because of the lack of information and description of the sample and the condition of the ship, e.g. the condition of the ship when it wrecked, how many tanks the ship has, how many tanks that broken such that the oil spilled out due to the accident, the placement of the oil spill in the collecting ships; therefore the author decided to use the same reference samples as used in SINTEF report.

The map of the samples location is shown in Fig.3.6 and 3.7. The maps were developed with the help of kart.finn.no based on tabulated data in Table 3.3. It shows sample locations along the west coast of Norway. It is merely approximate locations in order to give overview about the relative distance between the sample and the accident location. The relative distance is tabulated in Table 3.4.

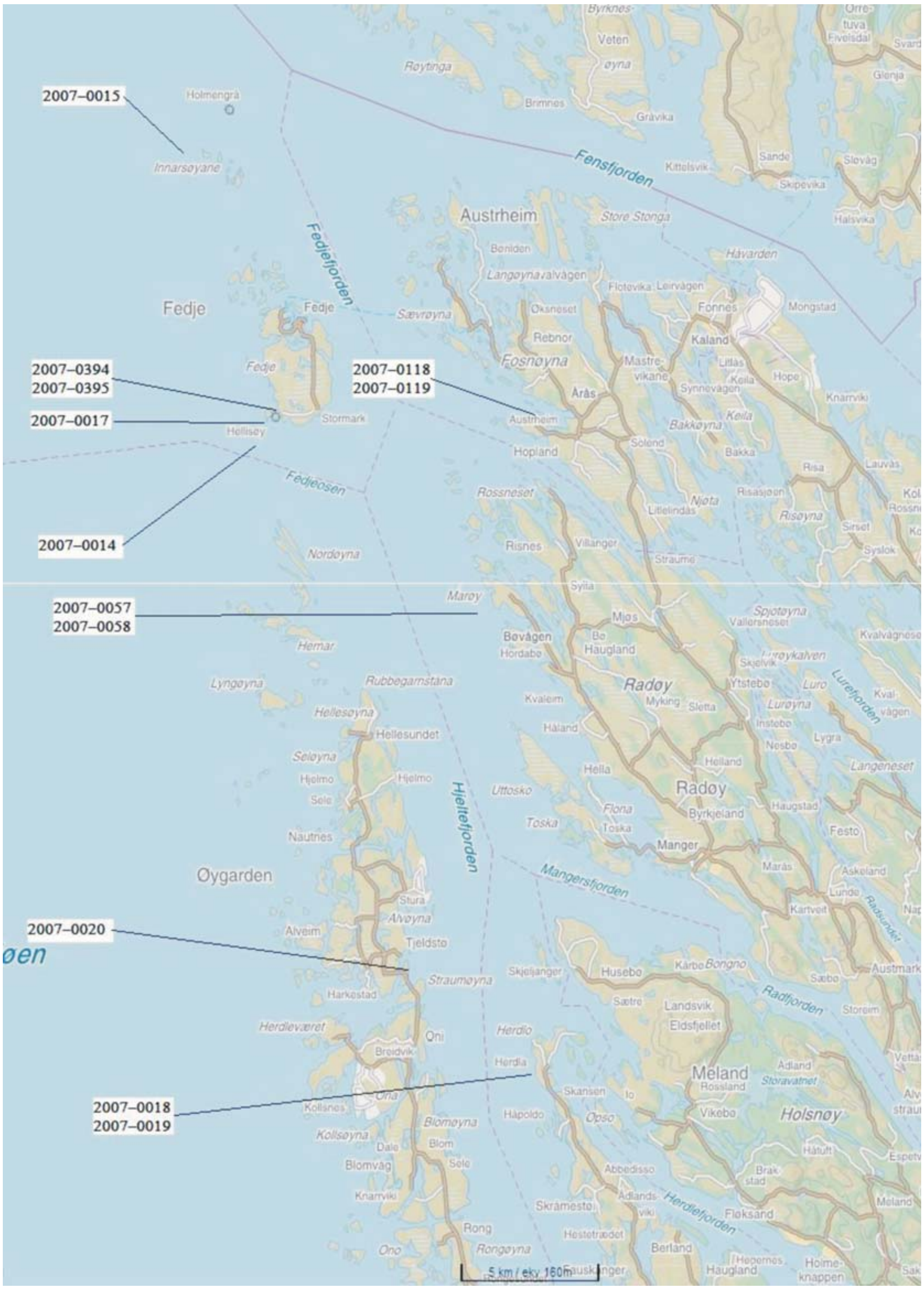

Figure 3.6: Approximate sample locations of the MS Server oil spill accident 1.

The author also received data of GC-FID chromatogram of the samples, the peak response of bio-marker and PAH compounds for each of the samples, and DRs generated from GC-MS response. The data was produced by SINTEF

Table 3.4: Relative distance of the sample locations to MS Server accident.

Location	SINTEF ID	Dist.(km)
Fedje	2007-0017, 2007-0394, 2007-0395	0
Innarøyene	2007-0015	8
Austrheim	2007-0118, 2007-0119	9
Radøy	2007-0057, 2007-0058	13
Sauøy	2007-0020	20
Herdla	2007-0018, 2007-0019	23
Flora	2007-0028, 2007-0029, 2007-0030	95
Vetvika	2007-0282	125
Gulen	2007-0059, 2007-0060, 2007-0061	125
Vågsøy	2007-0026, 2007-0027	145
Selje	2007-0025	165
Herøy	2007-0063	180
Sande	2007-0084	200
Ulstein	2007-0042, 2007-0065, 2007-0066, 2007-0067, 2007-0068.	205

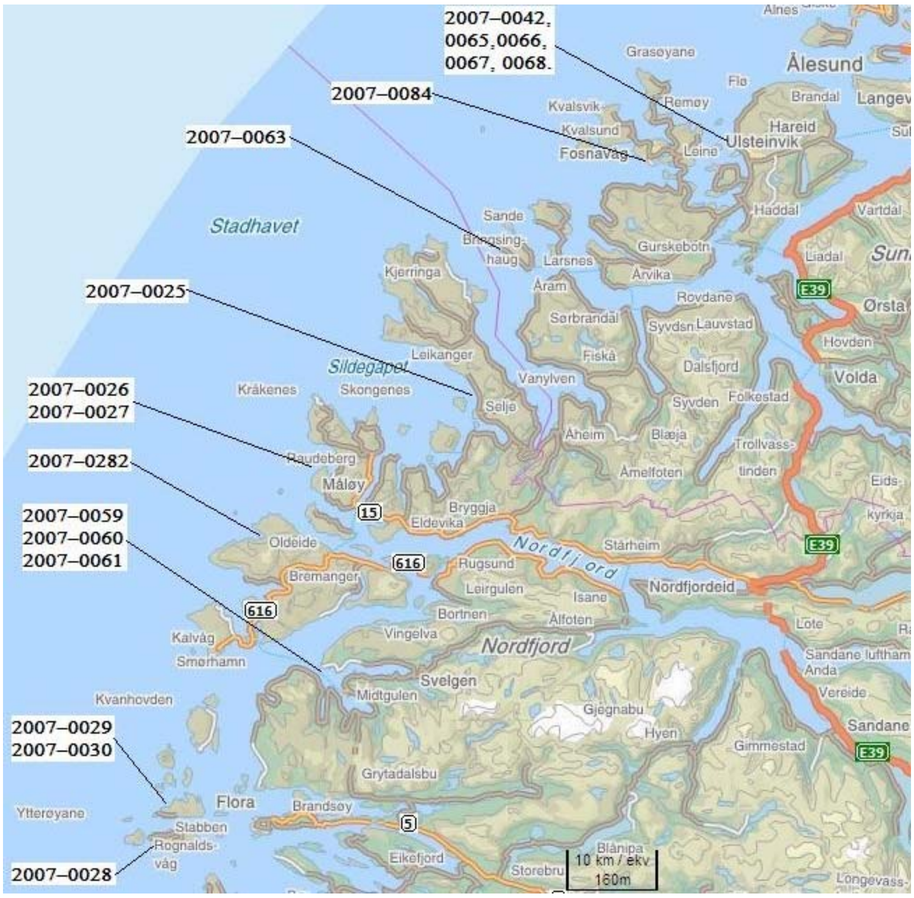

Figure 3.7: Approximate sample locations of the MS Server oil spill accident 2.

and the result of the corresponding fingerprinting was reported in Almås et al. [2007].

4 CEN UNIVARIATE METHOD APPLIED TO FULL CITY AND SERVER OIL SPILL

4.1 COVERAGE

Before addressing the multivariate problem, it is necessary to have complete understanding of the presently available univariate CEN-method. Therefore, this chapter focuses on the application of CEN-method (CEN/TR 15522-2) on the identification of sources for illegal oil spills. The method is implemented to the case of MS Server and MV Full City oil spills at Norwegian waters in 2007 and 2009 respectively.

As the basis for the investigation, SINTEF reports for both oil spill cases were made available as well as its supporting data. The main data needed for Level 1 (GC-FID) screening is the GC-FID chromatogram, which available in form of figures in pdf file. No digital data available. Therefore, effort has been given to digitize all GC-FID chromatogram of the samples by mean of graph digitizing software, *windig25*. Afterward, Level 1 screening by overlaying the chromatogram of the spill sample on top of the reference sample could be easily performed in *Matlab*. Hopefully any difference of chromatograms and n-alkanes distribution can be observed. If there is exist any difference, consideration should be made whether the differences are caused by weathering process or other reasons.

Primary weathering process after oil spill accident is evaporation. Thus, for oil spill investigation, spill samples could be stated weathered or not by seeing are they evaporated or not. A spill sample can be said evaporated if it fulfills two conditions as follows.

1. Concentration of low-boiling compounds is lower in the spill sample than in the sample taken from a suspected source.
2. In the case of compounds with otherwise similar weathering characteristics, the decrease in concentration is always more pronounced in those compounds with lower boiling points.

The main data needed for Level 2 (GC-MS) analysis is the response of biomarkers and PAHs. Most of the responses were available in excel file (*.xls) format. Thereafter, the author calculated the diagnostic ratios as suggested by CEN. It has been found some discrepancies in the calculation as compared to the ones calculated in the excel file provided by SINTEF. The reason is explained later in the discussion section. There was no responses of the biomarkers and PAHs for reference sample at Såstein (MV Full City case). Therefore, the author employed directly its diagnostic ratios, which available from the SINTEF report.

The second and third part of this chapter present the case study of MS Server and MV Full City oil spill respectively. Visual inspection of GC-FID, GC-MS fingerprinting and evaluation of diagnostic ratio, and the discussion of the results, as well as the comparison with the SINTEF reports are presented in the consecutive sub-sections.

4.2 SERVER

4.2.1 *Visual Inspection of Gas Chromatography and Flame Ionization Detection (GC-FID)*

The first level (Level 1) for oil spill investigation using CEN-method is GC-FID screening analysis. The GC-FID chromatograms data of spill samples are compared with the GC-FID chromatograms of the source samples by overlaying both chromatograms. In this case, samples with SINTEF ID 2007-0017,2007-0023,2007-0024,2007-0033 are used as references. This samples then will be overlayed with another spill samples to see whether they are different or not. Typical overlaying of the GC-FID chromatograms between the spill and reference samples is presented in Fig.4.1. The figure shows that there is shifting of retention time between the spill and reference taken from Fedje (SINTEF ID 2007-0017), tank 4 (SINTEF ID 2007-0024) and "KV Eigun" (SINTEF ID 2007-0033), which indicates that there is re-distribution of chemical composition. While overlaying with sample from tank 3 (SINTEF ID 2007-0023) shows no shifting. However, the spill sample tends to have higher concentration as compared to the reference sample. This is somehow interesting and need to be explained more.

The overlaying of the GC-FID chromatograms for all sample is presented in Appendix B and the conclusion is drawn in Table 4.1.

Table 4.1: Summary of result of overlaid GC-FID Chromatogram of "Server" oil spill samples.

ID	Ref 1*	Ref 2*	Ref 3	Ref 4
2007-0010	similar	similar	similar	similar
2007-0011	similar	similar	similar	similar
2007-0012	similar	similar	similar	similar
2007-0014	diferent	different	different	different
2007-0015	similar	similar	similar	similar
2007-0016	similar	similar	similar	similar
2007-0018	diw	diw	different	diw
2007-0019	similar	diw	different	similar
2007-0020	similar	diw	different	similar
2007-0021	similar	similar	different	similar
2007-0022	similar	different	different	different

Continued on Next Page...

ID	Ref 1*	Ref 2*	Ref 3	Ref 4
2007-0025	diw	diw	different	diw
2007-0026	similar	similar	different	similar
2007-0027	similar	similar	different	similar
2007-0028	similar	similar	different	similar
2007-0029	similar	similar	different	similar
2007-0030	similar	similar	different	similar
2007-0042	diw	different	different	diw
2007-0055	similar	similar	different	Similar
2007-0056	diw	different	different	diw
2007-0057	similar	different	different	similar
2007-0058	similar	diw	different	diw
2007-0059	similar	diw	different	Similar
2007-0060	similar	diw	different	Similar
2007-0061	similar	diw	different	Similar
2007-0062	different	different	different	different
2007-0063	diw	diw	different	diw
2007-0064	diw	diw	different	diw
2007-0065	diw	diw	different	diw
2007-0066	diw	diw	different	diw
2007-0067	diw	diw	different	diw
2007-0068	diw	diw	different	diw
2007-0069	diw	different	different	diw
2007-0070	different	different	different	different
2007-0084	diw	diw	different	diw
2007-0105	different	different	different	different
2007-0118	similar	similar	diw	similar
2007-0119	similar	different	different	diw
2007-0282	similar	diw	diw	Similar
2007-0394	diw	diw	different	diw
2007-0395	similar	diw	different	similar
*Note	Ref 1: comparison with SINTEF ID 2007-0017, Ref 2: comparison with SINTEF ID2007-0023, Ref 3: comparison with SINTEF ID2007-0024, Ref 4: comparison with SINTEF ID:2007-0033, diw:different-weathered			

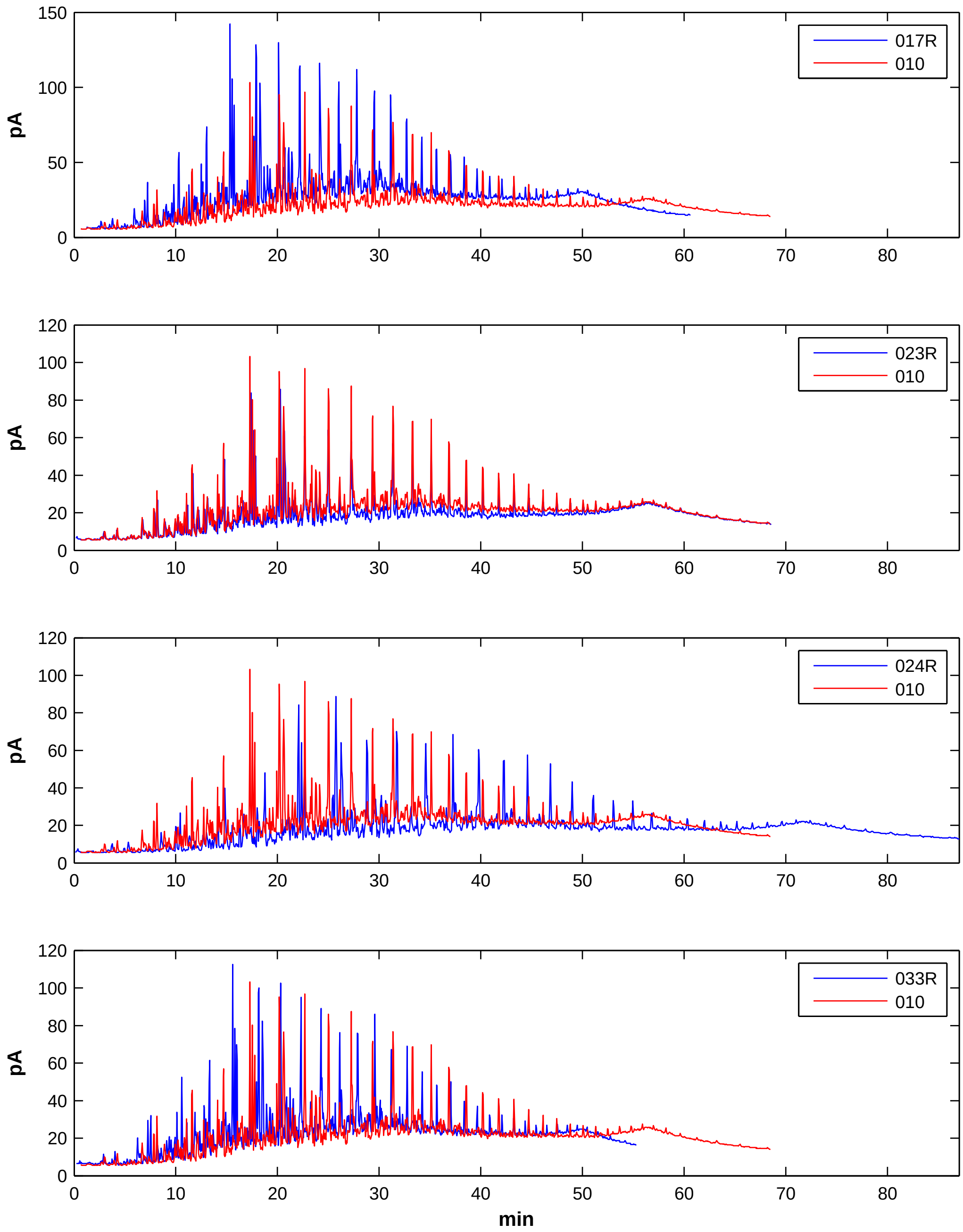

Figure 4.1: Overlaying of the GC-FID chromatograms of the oil spill sample (SINTEF ID: 2007-0010) and the reference samples.

4.2.2 *Gas Chromatography and Mass Spectrometry (GC-MS) Fingerprinting and Evaluation of Diagnostic Ratio*

The next level (Level 2) was GC-MS fingerprinting. The samples that continued to this level should be 41 samples because four samples were identified as non match at level 1. But the author only received diagnostic ratios data, which were generated from GC-MS responses for only 23 samples. From those 23 samples, some of them were analyzed several times. For example sample with SINTEF ID 2007-0017 and 2007-062 were analyzed three times, sample with SINTEF ID 2007-0022, 2007-0023 and 2007-0070 were analyzed twice. These duplications were used for evaluating the precision of the actual analysis series and the precision of the individual diagnostic ratios.

Those 23 samples analyzed using GC-MS also included SINTEF ID 2007-0014, 2007-0062, 2007-0070 and 2007-005. These samples should not be analyzed using GC-MS according to CEN-methodfor oil spill forensic because from the result of screening level indicated that they were different from the references and their differences were not caused by weathering.

Considering some backgrounds above, the author decided to do this level of analysis by using the data given by SINTEF without the data of the samples that should be ruled out, i.e data from 23 samples minus data from samples that different from references in the first level.

The data obtained from GC-MS analysis were responses of selected PAHs and biomarker compounds. These responses were used to calculate diagnostic ratio of each PAHs and biomarker compounds. Calculation of the diagnostic ratios was inaccordance with the recommendation given in the CEN-method for oil spill identification Part 2. Detailed calculated DR is provided in Appendix C. After calculating the diagnostic ratio of each sample, the diagnostic ratio of spill samples then to be compared with the diagnostic ratio of source/reference samples. The calculation of diagnostic ratio for each sample was done using *MATLAB*. Detailed evaluation of diagnostic ratio for "MS Server" oil spill is given in Appendix E.

The results of the evaluation of the GC-FID chromatogram from Level 1, the evaluation of the GC-MS chromatogram in Level 2, and the evaluation of the diagnostic ratios are summarized in Table 4.2. The table shows that samples with SINTEF ID no 2007-0014 (PadSample from sheen/rainbow oil film outside the lihgthouse at Fedje.), 2007-0062 (Oil on birds (gulls) Onøy, Lurøy), 2007-0070 (Bird feathers from wounded seagull (skårunge), Træna), and 2007-0105 (Oil sample from Eide, 9380 Gryllefjord) are concluded as non match because according to GC-FID chromatograms, they are different from the reference samples and the differences were not caused by weathering. Another sample that concluded as non match are oil sample from sandy beach Selje kommune, bird feathers from dead eiders (nr. 5), Osnessanden, Ulstein and oil sample from kelp and grass, Okstadvika, Herøy with SINTEF ID 20007-0025, 2007-0068, and 2007-0084, respectively. This oil sample has many diagnostic ratios that exceeded repeatability limit, i.e has many diagnostic ratio the different percentages more than 14%. The rest of the samples that have been analyzed until Level 2 can be concluded as probable match. This is because the samples have several diagnostic ratios that outside repeatability limit, but it can be explained by weathering.

Table 4.2: Summary of the results of MS Server oil spill fingerprinting.

ID	L1*	L2*	Concl	ID	L1*	L2*	Concl
2007-0010	X	-	*	2007-0011	X	-	*
2007-0012	X	-	*	2007-0014	X	X	NM
2007-0015	X	-	*	2007-0016	X	-	*
2007-0017	X	X	Ref	2007-0018	X	X	NM
2007-0019	X	X	PM	2007-0020	X	-	*
2007-0021	X	X	M	2007-0022	X	X	NM
2007-0023	X	X	Ref	2007-0024	X	X	Ref
2007-0025	X	X	NM	2007-0026	X	-	*
2007-0027	X	-	*	2007-0028	X	-	*
2007-0029	X	-	*	2007-0030	X	-	*
2007-0033	X	X	Ref	2007-0042	X	-	*
2007-0055	X	-	*	2007-0056	X	-	*
2007-0057	X	-	*	2007-0058	X	-	*
2007-0059	X	-	*	2007-0060	X	-	*
2007-0061	X	-	*	2007-0062	X	X	NM
2007-0063	X	X	PM	2007-0064	X	X	PM
2007-0065	X	X	PM	2007-0066	X	X	PM
2007-0067	X	X	PM	2007-0068	X	X	NM
2007-0069	X	-	*	2007-0070	X	X	NM
2007-0084	X	X	NM	2007-0105	X	X	NM
2007-0118	X	-	*	2007-0119	X	-	*
2007-0282	X	X	PM	2007-0394	X	X	PM
2007-0395	X	X	PM				

*Note. L1: Level 1, L2: Level 2, Concl: Conclusion

4.2.3 *Comparison with SINTEF's Result*

First of all, the author would like to comment regarding the procedure of the oil spill forensic as reported by Almås et al. [2007] in SINTEF report. They indicated that if the result of the Level 1 evaluation (i.e. visual inspection on the GC-FID) confirms of non match between the spill sample and the source sample due to non-weathering process, then the sample still goes to Level 2 evaluation (i.e. GC-MS). This practice seems to be difference from the CEN-method for oil spill identification Part 2. CEN documentation mentions that if the result of Level 1 evaluation confirms of non match between the spill sample and the source sample due to non-weathering process, then the spill sample can be concluded as non match and no further evaluation is needed.

CEN documentation also mentions that if the result of Level 1 evaluation confirms of match between the spill sample and the source sample, then the spill sample will be subjected to Level 2 evaluation. Almås et al. [2007] indicated the same way as what CEN documentation suggested, but most of the spill samples were end up at Level 1 only after being concluded as match with the source sample.

The author of this report believes that regardless of the limitation in time, money, and resources, all the spill samples need to be assessed with Level 1 and 2 evaluation before being concluded as match or non match. Of course, in reality those limitations force us to give priority, i.e. which sample goes for Level 1 only and which sample goes for Level 1 and 2. CEN documentation seems to be in favor for the oil spill suspects (ship owners, oil companies, etc) rather than the environmentalists and government or local population who suffers due to the oil spill. Whilst, Almås et al. [2007] shows the opposites. In this regard, the author expresses her support for the SINTEF approach.

Some of the conclusion are different as compared to the conclusion by Almås et al. [2007] in the SINTEF report for MS Server oil spill (see Table 4.3). For example, Almås et al. [2007] concluded oil sample from Stongholmsvikjo, Bømle kommune with SINTEF ID 2007-0064 as match. Almås et al. [2007] found that all of diagnostic ratio for this sample are below repeatability limit, while the author found that this sample still has diagnostic ratio that outside repeatability limit. Table 4.3 summarized the conclusion from SINTEF report [Almås et al., 2007].

Table 4.3: Summary of the results of MS Server oil spill fingerprinting by SINTEF.

ID	L1*	L2*	Concl	ID	L1*	L2*	Concl
2007-0010	X	-	M	2007-0011	X	-	M
2007-0012	X	-	M	2007-0014	X	X	NM
2007-0015	X	-	M	2007-0016	X	-	M
2007-0017	X	X	Ref	2007-0018	X	X	NM
2007-0019	X	X	M	2007-0020	X	-	M
2007-0021	X	X	M	2007-0022	X	X	NM
2007-0023	X	X	Ref	2007-0024	X	X	Ref
2007-0025	X	X	NM	2007-0026	X	-	M
2007-0027	X	-	M	2007-0028	X	-	M
2007-0029	X	-	M	2007-0030	X	-	M
2007-0033	X	X	Ref	2007-0042	X	-	M
2007-0055	X	-	M	2007-0056	X	-	M
2007-0057	X	-	M	2007-0058	X	-	M
2007-0059	X	-	M	2007-0060	X	-	M
2007-0061	X	-	M	2007-0062	X	X	NM

Continued on Next Page...

ID	L1*	L2*	Concl	ID	L1*	L2*	Concl
2007-0063	X	X	M	2007-0064	X	X	M
2007-0065	X	X	M	2007-0066	X	X	M
2007-0067	X	X	M	2007-0068	X	X	NM
2007-0069	X	-	no oil	2007-0070	X	X	NM
2007-0084	X	X	M	2007-0105	X	X	NM
2007-0118	X	-	PM	2007-0119	X	-	PM
2007-0282	X	X	M	2007-0394	X	X	M
2007-0395	X	X	M				

*Note. L1: Level 1, L2: Level 2, Concl: Conclusion

The other reason for the differences of SINTEF conclusion by Almås et al. [2007] and the author conclusion is on the selection of the diagnostic ratio. Some of diagnostic ratios recommended in CEN-method are not performed in SINTEF report, i.e DR-28ab, DR-25nor30ab, DR-Retene/C4phe, DR-TA21, and diagnostic ratio for sesquiterpanes. The reason for not included sesquiterpanes diagnostic ratios could be because of sesquiterpanes are optional and for samples that weathered, sesquiterpanes may not appear. DR-Retene/C4Phe was generated from retene, which is not specific for IFO oil type, therefor, DR-Retene/C4Phe also can not be used for "MS Server" oil spill fingerprinting. The reason why SINTEF did not include DR-28ab, DR-24nor30ab, and DR-TA21 could be because of the S/N of GC-MS chromatograms for these DRs were not qualify the criteria which has been determined by Al-Khudhairy [2006] in the CEN-method. This information was not available for the author since GC-MS chromatograms is only available in SINTEF report, which does not give clear profile.

The author also tried to compare the diagnostic ratio of spill sample with the single reference instead of compared it with the average diagnostic ratio of the reference sample. The intention of this was to find whether the comparison gives different conclusion. Even tough some diagnostic ratios evaluation in a spill sample were different when it was compared with the single source sample, overall diagnostic ratios drive the same conclusion as when it was compared with the average ratio of spill samples.

4.3 FULL CITY

4.3.1 *Visual Inspection of Gas Chromatography and Flame Ionization Detection (GC-FID)*

The visual inspection of GC-FID chromatograms of the ”MV Full City” samples was done with the same way as those for ”MS Server” samples. Typical of the overlaying process is shown in Fig.4.2. Detail overlaid GC-FID chromatograms of spill and source samples is presented in Appendix A.

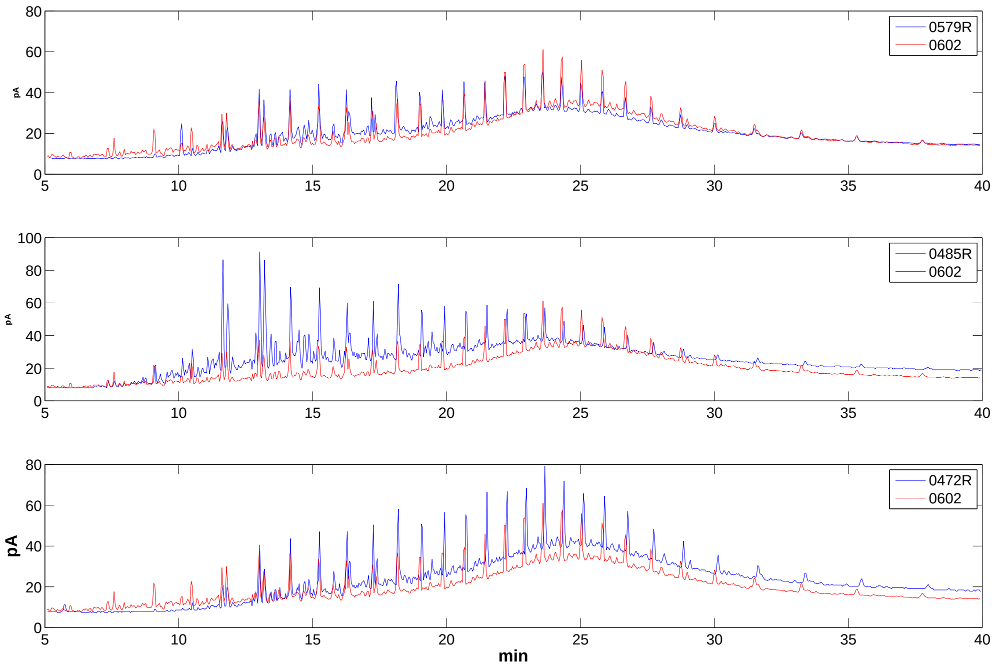

Figure 4.2: Overlaying of the GC-FID chromatograms of the oil spill sample (SINTEF ID: 2009-0602) and the reference samples.

The result in this level is summarized in Table 4.4. The table presents sample SINTEF ID no 2009-0473, 2009-0487, 2009-0494 and 2009-0624, which can be concluded as non match because they are different from the reference samples and the differences were not caused by weathering. Those samples than should be ruled out and eliminated from the next level. While the other samples should continue to the next level.

Table 4.4: Summary of result of overlaid GC-FID chromatogram of "Full City" spill samples.

ID	Ref 1*	Ref 2*	Ref 3
2009-0473	Different	different	Different
2009-0474	similar	similar	diw
2009-0482	similar	similar	diw
2009-0483	similar	similar	similar
2009-0484	similar	similar	similar
2009-0486	similar	similar	diw
2009-0487	Different	different	different
2009-0489	similar	similar	similar
2009-0490	similar	similar	similar
2009-0491	similar	similar	diw

Continued on Next Page...

ID	Ref 1*	Ref 2*	Ref 3
2009-0492	similar	similar	similar
2009-0493	diw	diw	diw
2009-0494	Different	Different	Different
2009-0495	similar	similar	similar
2009-0499	similar	similar	similar
2009-0500	diw	diw	diw
2009-0501	diw	diw	diw
2009-0518	similar	similar	similar
2009-0521	similar	similar	similar
2009-0522	similar	similar	similar
2009-0525	similar	similar	similar
2009-0602	similar	similar	similar
2009-0603	similar	similar	similar
2009-0604	similar	similar	similar
2009-0605	similar	similar	similar
2009-0606	diw	diw	diw
2009-0609	similar	similar	similar
2009-0614	diw	diw	diw
2009-0616	diw	diw	diw
2009-0622	diw	diw	diw
2009-0624	Different	different	Different
2009-0630	diw	diw	diw
2009-0634	diw	diw	diw
2009-0736	similar	similar	diw
2009-0737	similar	similar	diw

*Note,
Ref 1: comparison with SINTEF ID 2009-0472,
Ref 2: comparison with SINTEF ID2009-0579,
Ref 3: comparison with SINTEF ID2009-0485,
diw:different-weathered

4.3.2 *Gas Chromatography and Mass Spectrometry (GC-MS) Fingerprinting and Evaluation of Diagnostic Ratio*

According to CEN-method for oil spill identification, all samples that has the same pattern with the references or if there is any different, while the difference is caused by weathering, should continue to the next level of analysis, i.e GC-MS fingerprinting [Al-Khudhairy, 2006]. In this case, all samples except samples with SINTEF ID 2009-0473 and 2009-0487 should continue to the next level. Unfortunately, as happened in MS Server oil spill investigation, not all of the sample that should be analyzed in Level 2 was performed. The author only received 16 GC-MS data out of 37 samples. The non-match samples are not included in the GC-MS data.

The data obtained from GC-MS analysis are responses of selected PAHs and biomarkers compounds. These responses were used to calculate diagnostic ratio of each PAHs and biomarker compounds. Calculation of the diagnostic ratios was in accordance with the CEN-method for oil spill identification Part 2. The response of sample from Såstein is not given, so that the author did not calculate the diagnostic ratio of this sample for diagnostic evaluation, but use the diagnostic ratio of Såstein given by Faksness et al. [2010] in the SINTEF report.

After calculating the diagnostic ratio for each sample, the diagnostic ratio of spill samples then to be compared with the diagnostic ratio of source/reference samples. Calculated diagnostic ratios are given in Appendix C. There are some differences in the result of diagnostic calculation between the author calculation and SINTEF calculation. The differences occurred when calculating DR-C28 and DR-C29. These differences were because SINTEF calculation was not in accordance with CEN recommendation. According to the CEN recommendation, DR-C28 and DR-C29 should be calculated by $C28(R+S)/30ab$ and $C29(R+S)/30ab$, respectively. But in the SINTEF calculation sheet (excel file), DR-C28 and DR-C29 were calculated by $C28R/C28S$ and $C29R/C29S$, respectively.

The result of the evaluation of the GC-FID chromatogram in Level 1, GC-MS chromatogram in in Level 2, and the evaluation of the diagnostic ratios, the results can be summarized as shown in Table4.5. Detail evaluation of the diagnostic ratio of spill sample and reference samples can be seen in Appendix D.

Table 4.5: Summarized comparison of MS Full city oil spill sample and reference samples.

SINTEF ID	Comparison to Ref1*	Comparison to Ref.2*	Comparison to Ref.3*
2009-0472	match	Non match	Non match
2009-0473	Non match	Non match	Non match
2009-0474	*	*	*
2009-0482	*	*	*
2009-0483	*	*	*
2009-0484	*	*	*
2009-0485	Non match	Non match	match
2009-0486	Probable match	Probable match	Non match

Continued on Next Page…

SINTEF ID	Comparison to Ref1	Comparison to Ref.2	Comparison to Ref.3
2009-0487	Non match	Non match	Non match
2009-0489	Non match	Non match	Non match
2009-0490	*	*	*
2009-0491	Probable match	Probable match	Probable match
2009-0492	*	*	*
2009-0493	Non match	Non match	Non match
2009-0494	Non match	Non match	Non match
2009-0495	*	*	*
2009-0499	Probable match	Probable match	Non match
2009-0500	Probable match	Probable match	Probable match
2009-0501	match	Probable match	Probable match
2009-0518	*	*	*
2009-0521	*	*	*
2009-0522	*	*	*
2009-0525	*	*	*
2009-0579	Probable match	match	Non match
2009-0602	Probable match	Non match	Probable match
2009-0603	*	*	*
2009-0604	Probable match	Non match	Non match
2009-0605	*	*	*
2009-0606	Non match	Non match	Non match
2009-0609	Non match	Non match	Non match
2009-0614	Non match	Non match	Non match
2009-0616	Non match	Non match	Non match
2009-0622	Probable macth	Probable match	Non match
2009-0624	Non match	Non match	Non match
2009-0630	*	*	*
2009-0634	*	*	*
2009-0736	*	*	*
2009-0737	*	*	*
*Note	Reference 1: Oddane(2009-0472) Reference 2: Såstein (2009-0579) Reference 3: Krogshavn (2009-0485)		

4.3.3 *Comparison with SINTEF's Result*

Some conclusions given in Table 4.5 are different as compared to SINTEF's conclusion presented in the SINTEF report for "MV Full City" oil spill. Table 4.6 presents the conclusion from SINTEF report [Faksness et al., 2010].

Table 4.6: Summarized comparison of MV Full city oil spill sample and reference samples.

SINTEF ID	Comparison to Ref1*	Comparison to Ref.2*	Comparison to Ref.3*
2009-0473	non match	non match	non match
2009-0474	match	match	match
2009-0482	match	match	match
2009-0483	match	match	match
2009-0484	match	match	match
2009-0485	non match	non match	match
2009-0486	non match	match	non match
2009-0487	non match	non match	non match
2009-0489	non match	non match	non match
2009-0490	match	match	match
2009-0491	match	match	non match
2009-0492	match	match	match
2009-0493	non match	non match	non match
2009-0494	non match	non match	non match
2009-0495	match	match	match
2009-0499	match		
2009-0500	match		
2009-0501	match		
2009-0518	match	match	match
2009-0521	match	match	match
2009-0522	match	match	match
2009-0525	match	match	match
2009-0579	probable match	match	non match
2009-0602	non match	non match	non match
2009-0603	match	match	match
2009-0604	probable match	non match	non match
2009-0605	match	match	match
2009-0606	non match	non match	non match
2009-0609	non match	non match	non match
2009-0614	non match	non match	non match

Continued on Next Page...

SINTEF ID	Comparison to Ref1	Comparison to Ref.2	Comparison to Ref.3
2009-0616	non match	non match	non match
2009-0622	probable macth	probable match	non match
2009-0624	non match	non match	non match
2009-0630	match	match	match
2009-0634	match	match	match
2009-0736	match	match	match
2009-0737	match	match	match
*Note	Reference 1: Oddane(2009-0472)		
	Reference 2: Såstein (2009-0579)		
	Reference 3: Krogshavn (2009-0485)		

These differences were because, first, the author did not make any conclusion for some samples that according to GC-FID screening are match to the references. This was because Level 2 of analysis was not performed, whilst according to CEN-method, it must be performed. Faksness et al. [2010] concluded that these samples as match to the oil from "MV Full City". This could be because those samples were taken at the ship (cargoes and barges) and at the accident area (Såstein and area closest to Såstein, i.e. Mølen). This means no doubt that these samples were spilled oil from "MV Full City". Therefore, in order to save costs, etc. somehow GC-MS was not performed.

The other reason for the differences of Faksness et al. [2010] conclusion and the author's conclusion is on the selection of the diagnostic ratio of PAHs and biomarker compounds. Some of diagnostic ratios recommended in CEN methodology are not performed in SINTEF report i. e DR-C28, DR-C29, DR-C2829, DR-28ab, DR25nor30ab, DR-29ba, DR-Retene/C4-Phe and diagnostic ratios for Sesquiterpanes.

The reason for Faksness et al. [2010] report excluded DR-28ab and DR25nor30ab for evaluation could be because these diagnostic ratios were generated from 28,30-bisnorhopane and 25-norhopane. The response of GC-MS of these biomarkers in all reference samples is zero. These mean 28,30-bisnorhopane and 25-norhopane markers are not available in all of the reference samples.

The reason for sesquiterpanes were excluded for the evaluation is also understandable. Sesquiterpanes are optional biomarkers for oil spill identification. The use of sesquiterpanes only valid if the samples are not weathered. This is because sesquiterpane has low boiling point and can be easily evaporated.

The reason for DR-Retene/C4-Phe were excluded for the evaluation could be because "MV Full City" containing IFOs oil type. In this type, retene should be not appears because it is an aromatics with slightly longer side chains that are not produced in higher-temperature processes. Therefore, this DR is not source specific [Al-Khudhairy, 2006].

The reason for Faksness et al. [2010] excluded DR-28ab, DR25nor30ab, DR-TA21 and DR-Retene/C4-Phe in the analysis could be because of the S/N of GC-MS chromatograms for these DRs are not fulfilled the criteria which has been determined by Al-Khudhairy [2006] in the CEN method. This information as not available for the author since GC-MS chromatograms was only available in SINTEF report by Faksness et al. [2010] which did not give clear profile.

5 PRINCIPAL COMPONENT ANALYSIS

5.1 GENERAL

In the previous chapter, CEN-method for oil spill investigation has been applied for "MV Full City" and "MS Server" oil spill cases. There are some discrepancies between the author's conclusion and SINTEF's conclusion. These discrepancies may be because CEN-methods and other univariate methods for oil spill investigation are heavily relied on skill and expertise of the analyst. Another reason is because crude oils and petroleum products are complex mixtures of chemical compounds, so it is not sufficient to analyze the oil spill phenomenon by using univariate approach [Wang and Scout, 2007]. Moreover, CEN-method for oil spill investigation mentions that the multivariate analysis, such as PCA, may be performed as an alternative approach on evaluating the diagnostic ratios between multiple samples [Al-Khudhairy, 2006].

The objective of oil spill investigation is to discover whether an oil spill sample matches to the reference (source/suspect) or not. The PCA is able to find the relationships between objects or finding classes of similar objects, such that we know which object is not belonging to the classes [Wold, 1990]. In oil spill forensic case, a sample that lays far from any clustered reference samples means not match to the reference (source/suspect) samples. Another advantage of using PCA for oil spill investigation is its ability to determine which variables (diagnostic ratios) that contribute to a class. It is useful to investigate whether an oil has been subjected to weathering process or not. In this work, PCA was performed with a multivariate statistical analysis software called *Unscrambler*.

This PCA was conducted to the diagnostic ratios data which was generated from GC-MS chromatograms performed by SINTEF. Therefore, not all of the samples were included in PCA because not all samples were analyzed using GC-MS. Detailed DRs data can be seen in Appendix C.

All variables to be used in this analysis has been selected in order to evaluate heterogeneity and analytical variation based on Stout's suggestion [Stout et al., 2001]. See Fig.2.4. The method excluding DRs of triplicate sample which has RSD greater than 5%. Both of DR data from "MV Full City" and "MS Server" oil spill cases contain number of samples which are smaller as compared to the number of variables. Therefore, cross validation was applied [CAMO, 2006].

As comparison, PCAs were performed on the data sets, either with or without autoscaling the variables. By autoscaling the variables, each element in the X-matrix is divided by its standard deviation. This will make each autoscaled variable get the same variance and therefore, give them the same chance to influence the estimation of the principal components [CAMO, 2006]. Otherwise, performing PCA without autoscaling the variables also give advantages.

Especially when a variable has small variance and this variable is a noisy variable. Dividing this variable with it's standard deviation will increase the impact of noise in the model [Esbensen et al., 1994].

5.2 PRINCIPAL COMPONENT ANALYSIS APPLIED TO "FULL CITY"OIL SPILL CASE

Evaluation of GC-MS chromatograms of the selected samples shows some target analytes that are relevant for the analysis. Available data (i.e. diagnostic ratios) is presented in Appendix C. These diagnostic ratios were provided by SINTEF and were not directly calculated from GC-MS data. In addition, the diagnostic ratios of sample from Såstein sample (that were used for reference sample and triplicate analysis) were not adopted from SINTEF's report [Faksness et al., 2010], as shown in the Table 5.1. For comparison, samples taken from Rockness accident, i.e sample Rockness and Askøy were also included in the data set.

Some samples contain missing value in some variables, i.e. C28 Tricyclic, C29 Tricyclic, C28+29 tricyclic, 28ab, 25nor30ab, 30G, retene/C4-Phe, SES1/SES2, SES3/SES5, SES4/SES9, SES5/SES10. These missing values also appear in the reference sample, i.e. sample from Såstein. This mean that these DRs are not source specific, such that they are not valid for analysis and should be eliminated.

Evaluation of DR in order to asses the heterogeneity and analytical variation showed that DR 30O, 29ba, TA21, and C2-dbt/C2-Phe have RSDs greater than 5%, so that those DRs should be eliminated from further numerical analysis (see Table 5.1).

5.2.1 *Principal Component Analysis Without Autoscaling the Variables*

Performing PCA without autoscaling means all calculation are based on the raw variables. This computation is useful if we want to see contribution of each variable in the model. This computation also useful when a variable has small variance and this variable is a noisy variable. Dividing this noisy variable with it's standard deviation will increase the impact of noise in the model [Esbensen et al., 1994].

Several PCAs were conducted to the selected diagnostic ratios from entire sample set. The results are shown in Fig.5.1 - 5.6. Fig.5.1 is the score plot of PCA conducted to all samples. The figure shows two samples that lay far from others. These samples were taken from Rockness and Askøy. This mean all samples taken after "MV Full City" casualty is different from sample from Rockness accident, i.e Rockness and Askøy. This also supported by Hotelling T2 view shown in Fig.5.2.

Loading plot of this PCA, Fig.5.3, shows that variable B(a)F/4-Mpy has high contribution on sample from Askoy and variable C3-dbt/C3-Chr has high contribution on sample from "Rockness". These variables distinguished those two sample from oil samples taken from "Full City" accident.

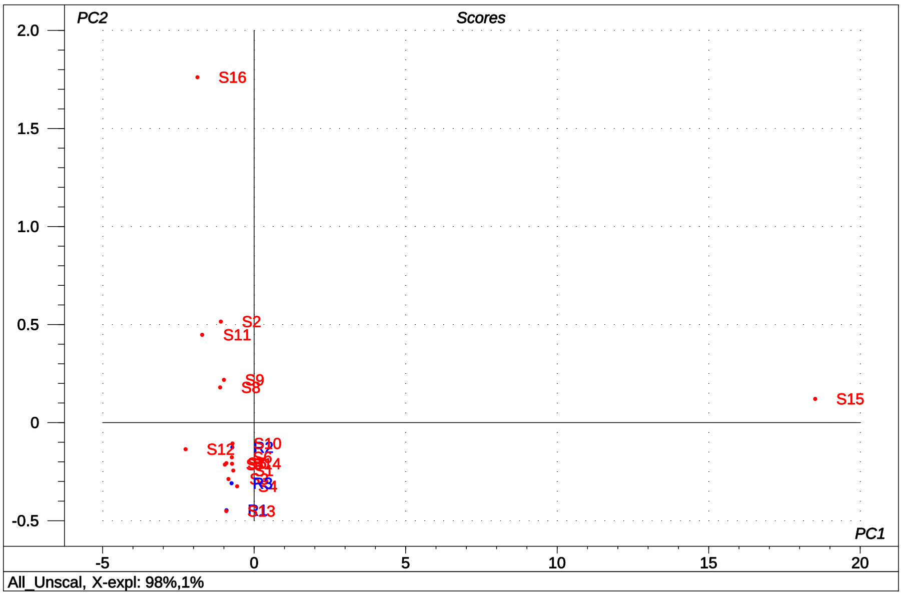

Figure 5.1: Score Plot PCA performed on all of the sample from "Full City" accident. See Table 5.2 for remarks.

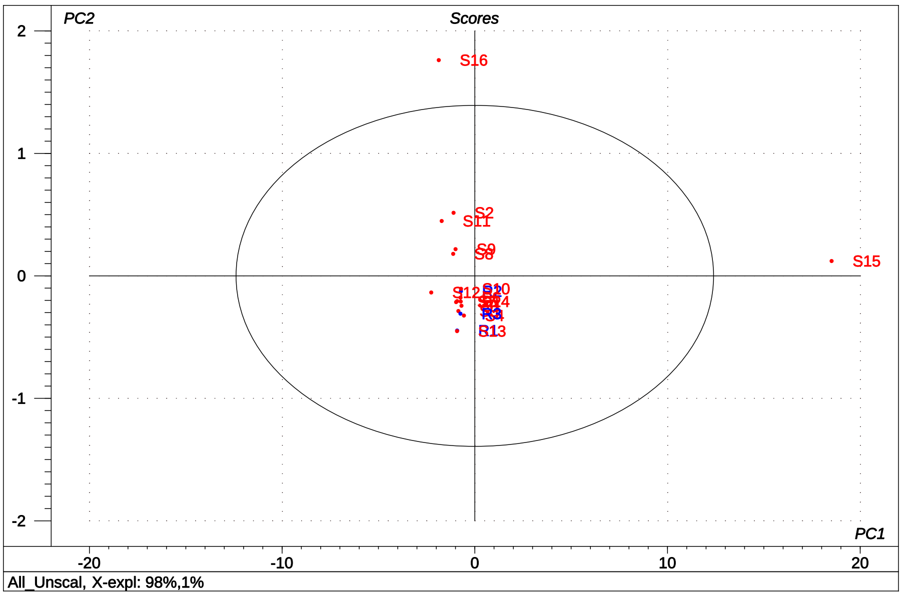

Figure 5.2: Hotelling T2 view of all sample from "Full City" accident. See Table 5.2 for remarks.

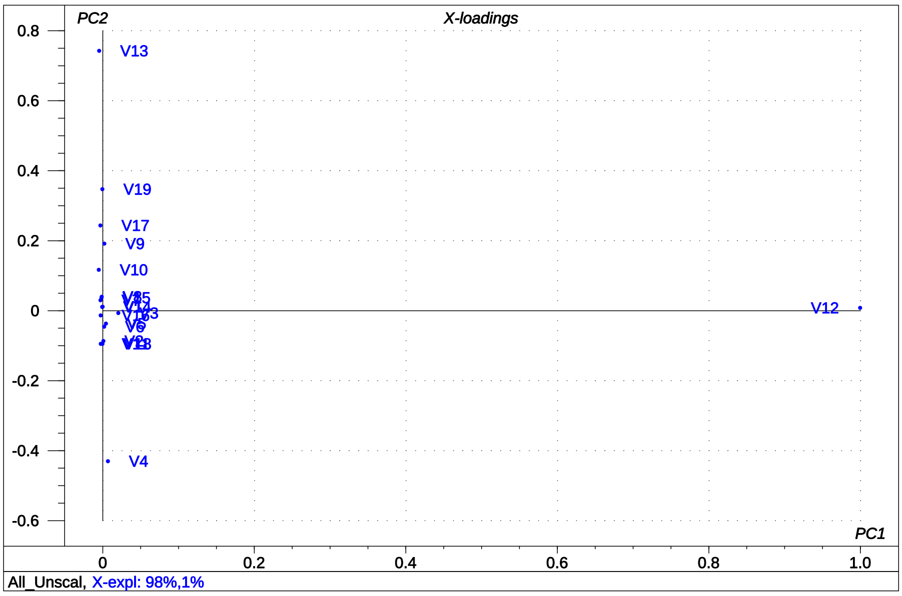

Figure 5.3: Loading Plot PCA performed on the data uses for "Full City" Oil Spill Identification without scaling the variables. See Table 5.2 for remarks.

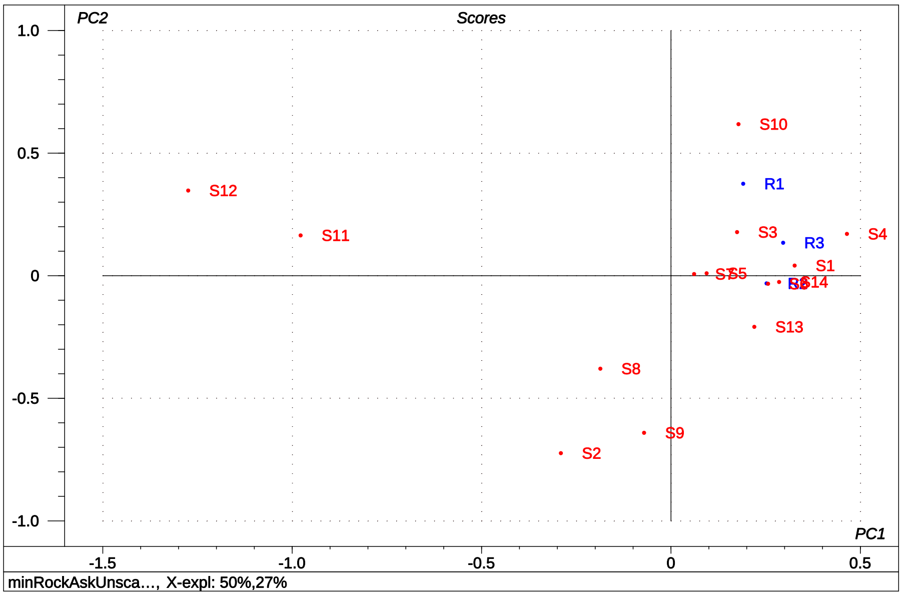

Figure 5.4: Score Plot PCA performed on the data from "Full City" accident without sample from Åskoy and Rockness. See Table 5.2 for remarks.

Table 5.1: Diagnostic ratios value of triplicate sample ("Full City" oil spill case).

SINTEF ID	Såstein 0308	Såstein 0508	Såstein 1008	Mean	STD	RSD
27Ts	0.47	0.47	0.51	0.48	0.02	4.78
29ab	0.70	0.71	0.72	0.71	0.01	1.41
29Ts	0.14	0.13	0.13	0.13	0.01	4.33
30d	0.04	0.04	0.04	0.04	-	-
30O	0.05	0.06	0.04	0.05	0.01	20.00
29ba	0.06	0.06	0.07	0.06	0.01	9.12
29aaS	0.92	0.88	0.88	0.89	0.02	2.59
29bb	1.32	1.29	1.34	1.32	0.03	1.91
27bbSTER	0.52	0.52	0.51	0.52	0.01	1.12
28bbSTER	0.38	0.36	0.39	0.38	0.02	4.06
29bbSTER	0.62	0.64	0.63	0.63	0.01	1.59
TA21	0.58	0.50	0.50	0.53	0.05	8.77
TA26	0.41	0.44	0.45	0.43	0.02	4.80
TA27	0.96	0.91	0.88	0.92	0.04	4.41
2-MPIl-MP	2.12	2.14	2.10	2.12	0.02	0.94
4-MD/1-MD	2.55	2.58	2.59	2.57	0.02	0.81
C2-dbt/C2-phe	0.37	0.42	0.39	0.39	0.03	6.40
C3-dbt/C3-phe	0.53	0.54	0.51	0.53	0.02	2.90
C3-dbt/C3-chr	2.28	2.40	2.41	2.36	0.07	3.06
B(a)F/4-Mpy	0.38	0.39	0.41	0.39	0.02	3.88
B(b+c)F/4-Mpy	0.20	0.19	0.21	0.20	0.01	5.00
2Mpy/4-Mpy	1.06	1.07	1.05	1.06	0.01	0.94
l Mpy/4-Mpy	0.91	0.92	0.91	0.91	0.01	0.63

Sample from "Rockness" and "Askøy" are therefore not relevant for investigation of "Full City" oil spill case and should be removed for the next PCA. Fig.5.4 shows the score plot of PCA after removing sample from Rockness and Askøy. In this figure we can see none of the spill samples match with any type of heavy bunker oil (IFO180 and LS180) samples. Spilled samples seem to be a mixture of oil taking from machine room, barges and cargo tanks.

Loading plot in Fig.5.5 shows highly contribution of variable (Ba)F/4-Mpy to the samples from the ship barge and cargo. Variable 2-MP/1-MP gives high contribution on sample taken from machine room. This DR is useful to differentiate diesel oils and heavy bunker fuel oil. The loading plot gives information that oil in the machine room is strongly affected by DR 2MP/1MP. This means oil in the machine room contain more methyl-phenanthrenes as compared to the oils in the cargoes.

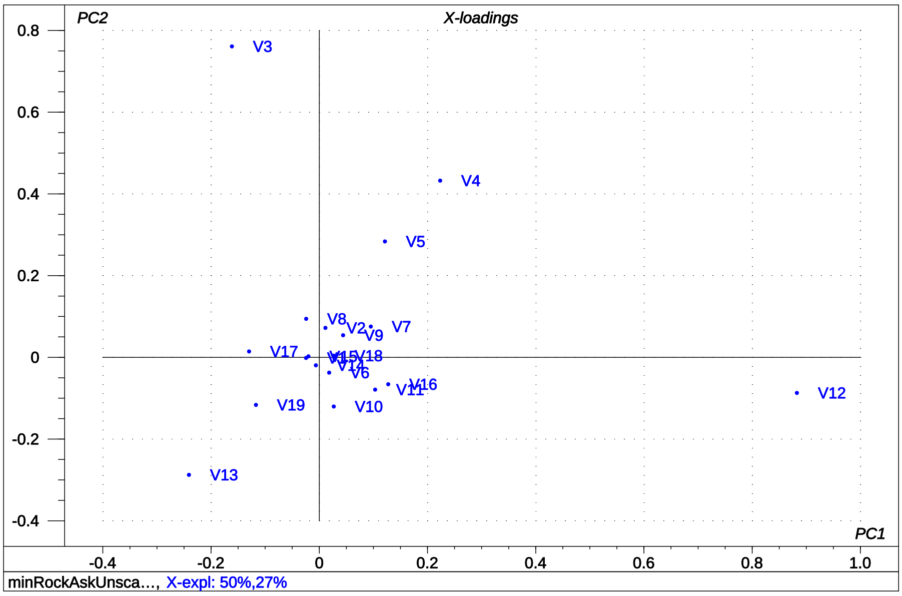

Figure 5.5: Loading Plot of PCA performed on the data from "MV Full City" accident without sample from Askøy and Rockness. See Table 5.2 for remarks.

PCA was then performed on the data by removing samples from machine room, barge samples, IFO 180 Vysotsk, HS 180 Skagen, and LS 180 Skagen. In this case, samples from Såstein, Oddane and Krogshavn have been chosen as reference samples [Faksness et al., 2010]. Fig.5.6 shows the score plot of this PCA. This figure is not easy to interpret by the author. The objection of this PCA is to see the tendency of a sample match to one of the reference sample. Whilst, this figure still not showing any cluster clearly. Therefore, another classification method should be applied to suggest the right conclusion.

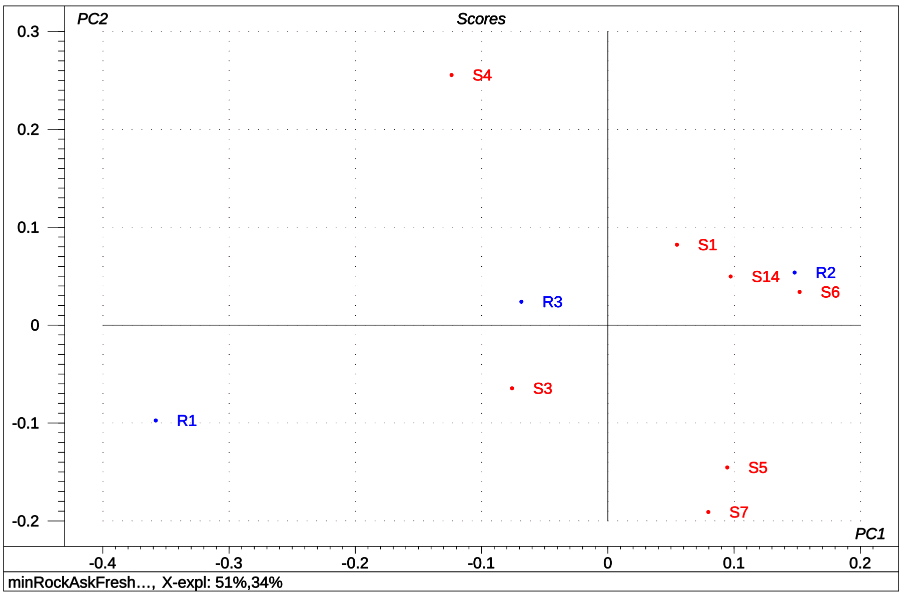

Figure 5.6: Score Plot PCA performed on only spill samples from "MV Full City" accident. See Table 5.2 for remarks.

Table 5.2: Remark for "Full City" Case

Remark	Sample	Remark	Variable name
R1	Krogshavn	V1	30d
R2	Oddane	V2	1 Mpy/4-Mpy
R3	Såstein	V3	4-MD/1-MD
S1	Mandal	V4	2-MPIl-MP
S2	Lekter	V5	2Mpy/4-Mpy
S3	Nevlunghavn	V6	27bbSTER
S4	Langesund bad	V7	29ab
S5	Grimstad	V8	29bbSTER
S6	Risor	V9	29bb
S7	Arendal	V10	29aaS
S8	Lasterom2	V11	C3-dbt/C3-phe
S9	Lasterom 4	V12	C3-dbt/C3-chr
S10	Maskinrom	V13	B(a)F/4-Mpy
S11	IFO180Vysotsk	V14	28bbSTER
S12	LS180 Skagen	V15	29Ts
S13	HS180 Skagen	V16	TA27
S14	Lillesand	V17	27Ts
S15	Rockness	V18	TA26
S16	Askøy	V19	B(b+c)F/4-Mpy

5.2.2 *Principal Component Analysis With Autoscaling the Variables*

Autoscaling or weighting variables by dividing each element in the **X**-matrix with its standard deviation. This method gives all variable, in this case DRs, the same chance to influence the model. This is used because several variables have different range. For example, variable 30d has value from 0.001-0.010, while variable 2-MP/1-MP ranged from 1-2.

The result of this PCA methods are shown in Fig.5.7-5.13. Fig.5.7 shows sample from Askøy which lays far from other samples. This is consistent with the one performed without autoscale the variables. Since sample from Askøy was taken from "Rockness" accident, this sample can be concluded as not match with oil from "MV Full City" accident and then was removed for the next PCA run. However, sample from "Rockness" (which is non match in the PCA run without autoscaled), in this PCA run seem to show sign of match with "MV Full City" accident. This is interesting since in fact sample from "Rockness" was not part of "MV Full City" accident. This could be because oil from "Rockness" and "Full City" were similar, i.e IFO 380. The loading plot, Fig5.8, shows that all variables have similar contribution to the model.

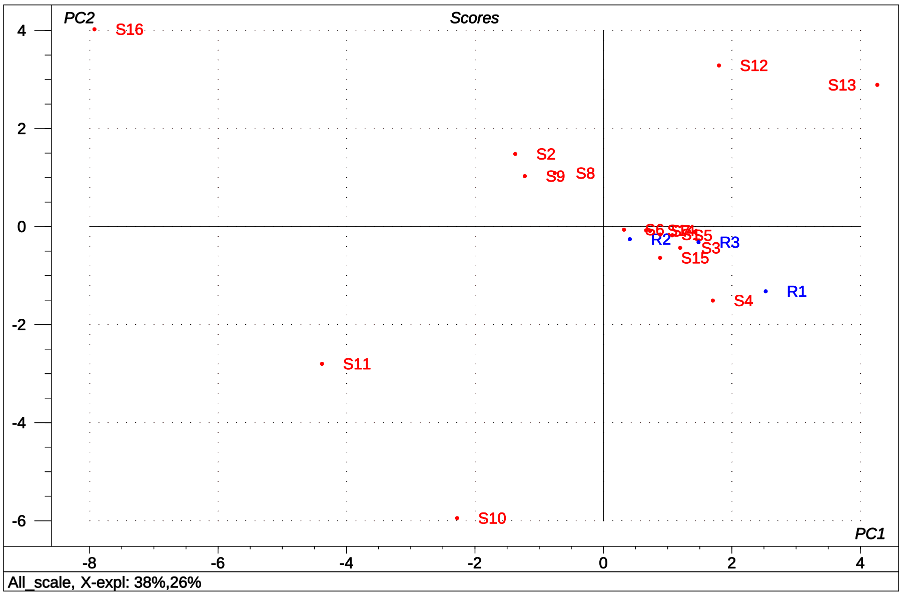

Figure 5.7: Score plot PCA performed on all sample uses for "Full City" oil spill identification, all variables are weighting with 1/STD. See Table 5.2 for remarks.

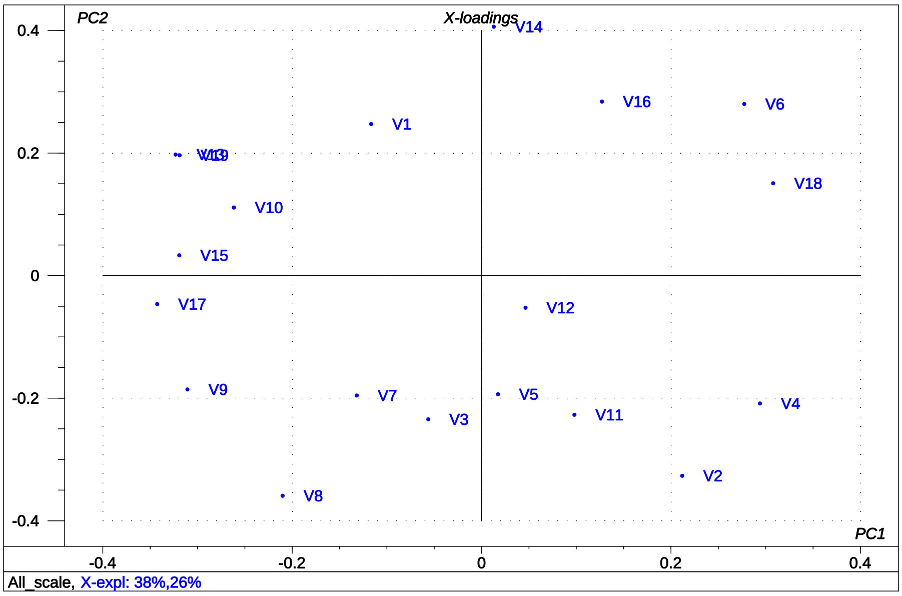

Figure 5.8: Loading plot PCA performed on all sample uses for "Full City" oil spill identification, all variables are weighting with 1/STD. See Table 5.2 for remarks.

Result of PCA run after removing this sample can be seen in Fig.5.9. This figure gives information that spilled oil samples form a linear line cluster. Sample taken from the ships cargoes and barges are located on the top of the line, whilst samples taken from the spilled area are located on the bottom of the line. Other samples, i.e sample taken from machine room and heavy bunker oil (IFO180, HS180 and LS180) seems to be different from spilled samples taken from the ship and the accident area.

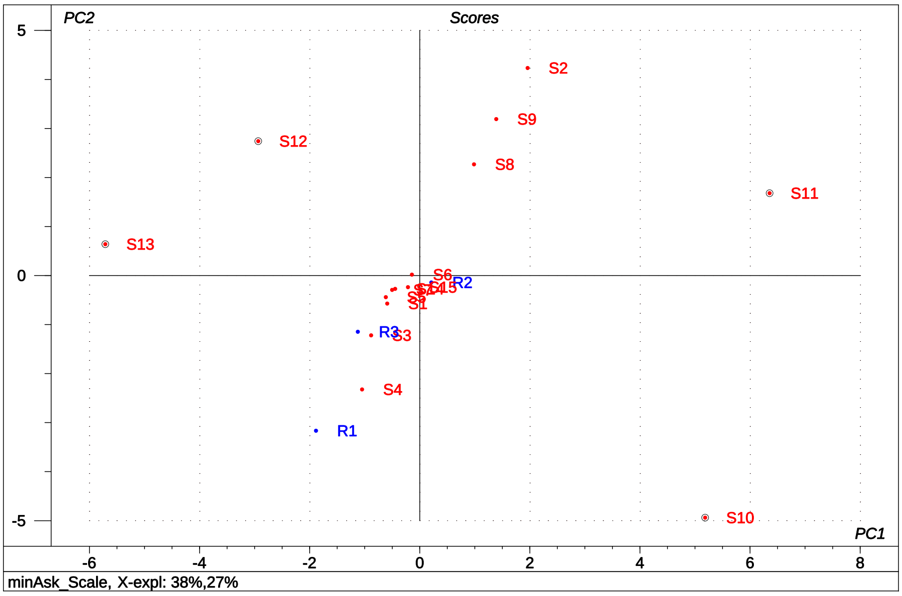

Figure 5.9: Score plot PCA performed on "MV Full City" oil spill DR data without sample from Askøy. All variables are weighting with 1/STD. See Table 5.2 for remarks.

It is interesting to see the behavior of "MV Full City" oil spill sample by removing these different samples for the next PCA run. The score plot is shown in Fig.5.10. In this figure, sample taken from "Rockness" appears as non match to oil from "Full City". This sample is then removed from the next analysis.

The score after removing "Rockness" is shown in Fig.5.11. This figure shows interesting pattern. Samples taken from the ship lay on negative direction on PC1, while samples taken on the spill area lay on positive direction on PC1. The biplot shown in Fig.5.12 tells us that some variables with higher ion mass (m/z), e.g. V18(TA 26) and V16 (TA 27), tend to lay on the right side of PC1. These variables are close to samples taken from the spilled areas. This mean that samples taken from spill area were more subjected to the weathering process as compared to the samples taken from the barges or cargoes. Samples taken at later date after accident, such as S4 (sample taken from Langesund bad at 7th August 2009), was more subjected by weathering processes as compared to the sample taken at earlier date, such as S6 (sample taken from Risør at 1st August 2009).

In order to obtain information about the behavior of oil after spilled, oil samples taken from the barges and cargoes were then removed from the next PCA run. Samples from Såstein, Oddane and Krogshavn have been chosen

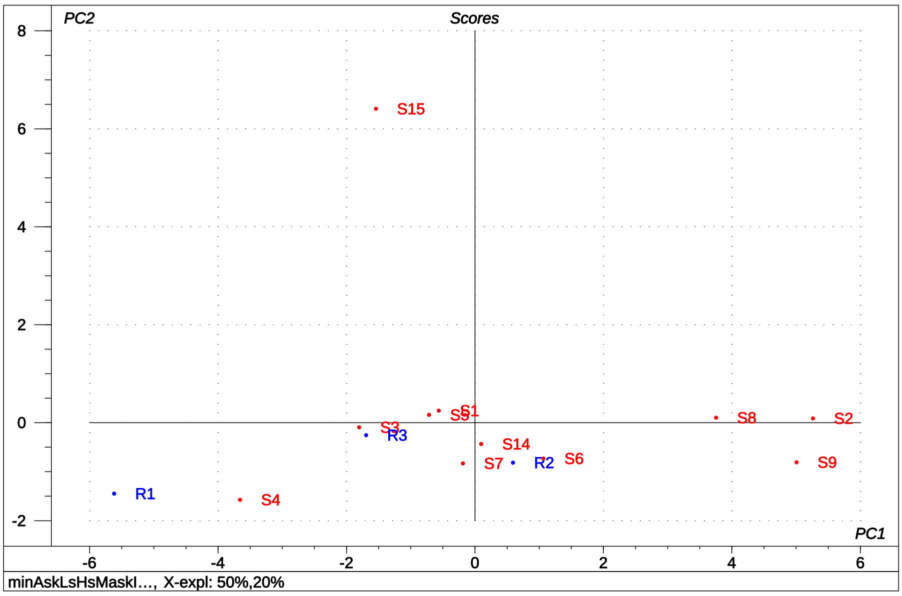

Figure 5.10: Score plot PCA performed on "MV Full City" oil spill DR data without sample from Askøy, IFO 180, HS180, LS180 and oil sample from machine room. All variables are weighting with 1/STD. See Table 5.2 for remarks.

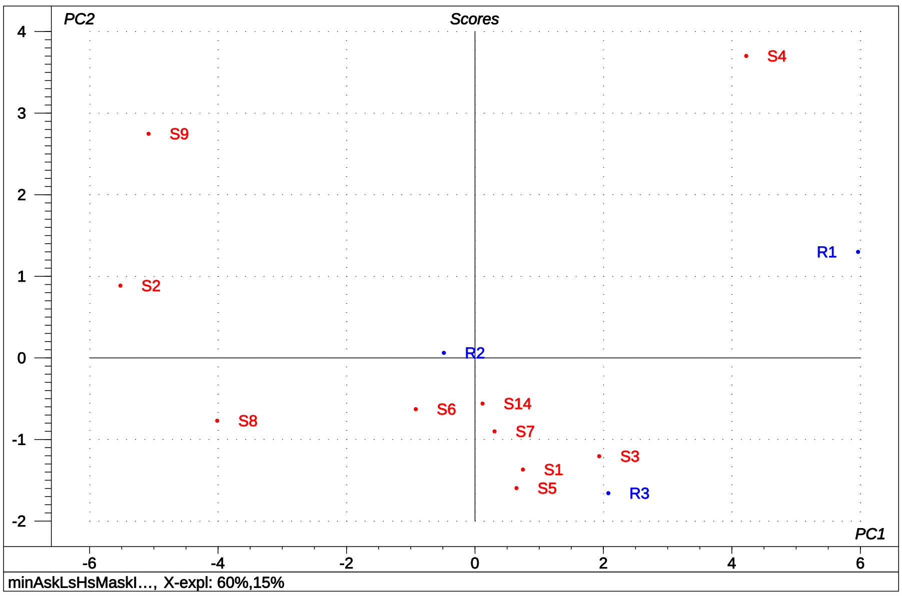

Figure 5.11: Score plot of PCA performed on "MV Full City" oil spill DR data without sample from Askøy, IFO 180, HS180, LS180, oil sample from machine room and "Rockness. All variables are weighting with 1/STD. See Table 5.2 for remarks.

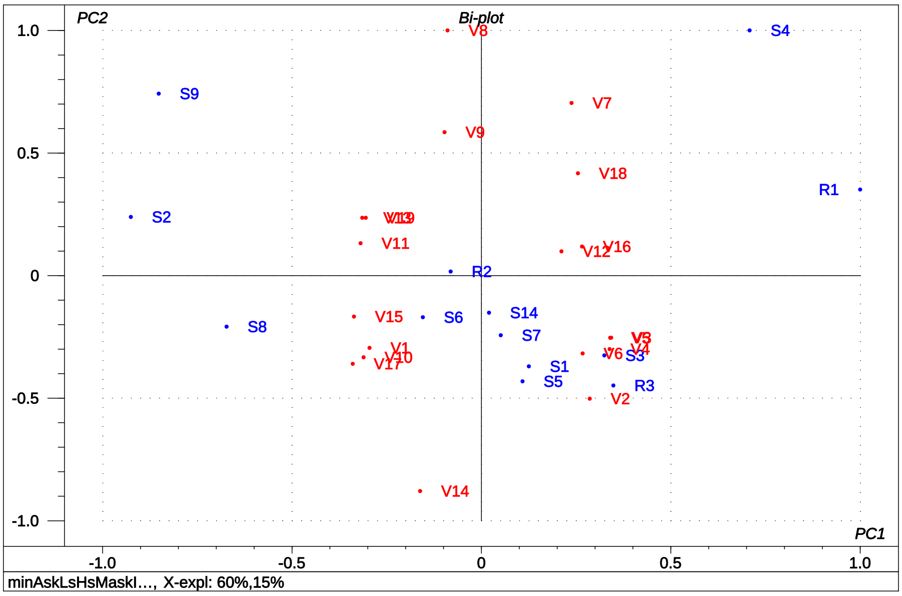

Figure 5.12: Biplot of PCA performed on "MV Full City" oil spill DR data without sample from Askøy, IFO 180, HS180, LS180, oil sample from machine room and "Rockness". All variables are weighting with 1/STD. See Table 5.2 for remarks.

as reference samples [Faksness et al., 2010] for this PCA. The score plot of this PCA, given in Fig.5.13 is not easy to interprets by the author. It seems the figure contain three clusters. The first cluster matches to reference oil from Oddane, the second cluster matches to reference oil from Såstein, and the last cluster match to reference oil from Krogshavn. This is in agreement with SINTEF's report which applied CEN-method for oil spill investigation [Faksness et al., 2010].

5.3 PRINCIPAL COMPONENT ANALYSIS APPLIED TO "MS SERVER"OIL SPILL CASE

In this case, oil sample from Fedje, KV eigun, tank 3 and tank 4 of MS Server are chosen as reference samples [Almås et al., 2007]. The diagnostic ratios were provided by SINTEF and can be seen in Appendix C. Some samples contain missing value in some variables, i.e. SES1/SES2, SES3/SES5, SES4/SES9, SES5/SES10.

Variable DR SES1/SES2 also has missing value in the references samples taken from tank 3 and tank 4 MS Server. It means that this DR is not source specific. Thus, DR SES1/SES2 can not be used for oil spill finger printing. The others variables, i.e. SES3/SES5, SES4/SES9, and SES5/SES10 mostly missing in the bird feathers samples. This indicates that these variables have been subjected by weathering processes. Therefore, these variable are also not suitable for oil spill finger printing. In order to evaluate analytical variance and weathering/heterogeneity, relative standard deviation of DR of triplicate samples are calculated. The triplicate sample is sample with ID 2007-017 from

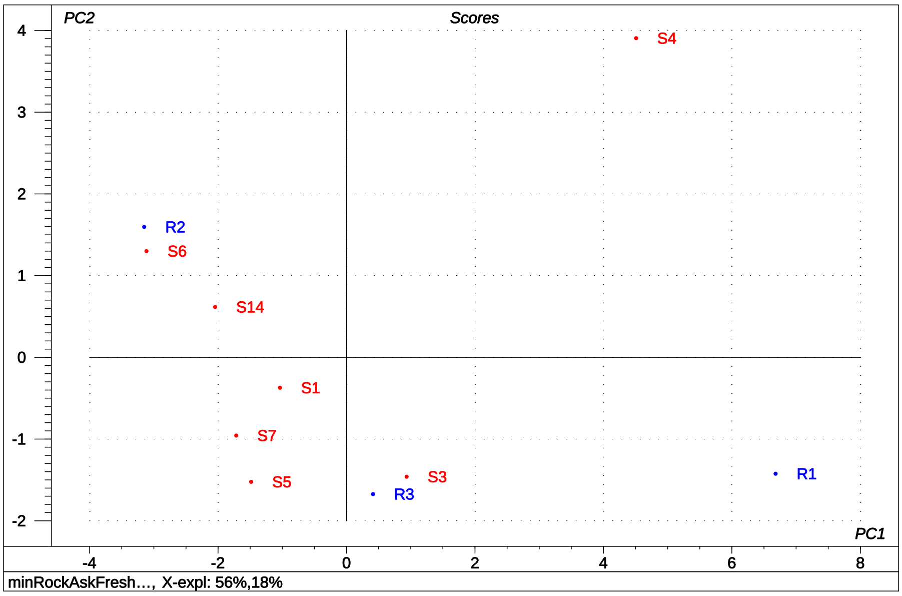

Figure 5.13: Score plot PCA performed on "MV Full City" oil spill DR data without sample from Askøy, barges, cargoes, machine room, IFO 180, HS180, LS180, and "Rockness". All variables are weighting with 1/STD. See Table 5.2 for remarks.

Fedje. The calculation is shown in the Table 5.3. As shown in Table 5.3, DR 30O, 29Ts, Retene/C4-phe, C3-dbt/C3-chr, 29aaS, C28tricycllics, 25nor30ab, C28+C29tricyclics, C29 tricyclics, 30d, and DR 28ab have RSD greater than 5% percent, therefore, this DRs should be removed for the analysis.

5.3.1 *Principal Component Analysis Without Autoscaling the Variables*

By performing PCA without autoscaling the variables, all calculations were based on the raw value of the variables. This computation is useful if we want to see contribution of each variable in the model. Some variables also have small variance, for example 29ab, 29ba, 30G and 27Ts. If these variable are noisy variables, dividing these variables with their standard deviation will increase the noise impact in the model [Esbensen et al., 1994].

Several PCAs are performed on the selected diagnostic ratio index from the entire sample sets without autoscaling the variables. The result is shown in Fig.5.14-5.18 Fig. 5.14 shows some samples form a cluster. This clustered samples contain reference samples. Some samples lay far from clustered sample are also detected. These samples are oil sample from Gryllefjord, teflon pad sample taken at Fedje, and bird Feather samples taken from Træna, and Lurøy. The composition of these samples also can not be easily explained by the variables in the biplot. See Fig.5.15. Fig.3.7 shows the location of the samples that quite far to the north from the accident area. Therefore, these samples are concluded as non match to the references samples and should be removed from the next PCA.

Table 5.3: Diagnostic ratios value of triplicate sample (sample from Fedje ID 2007-0017).

SINTEF ID	2007-0017	2007-0017	2007-0017	mean	STD	RSD
C28tricycllics	0.22	0.2	0.24	0.22	0.02	9.02
C29 tricyclics	0.16	0.15	0.19	0.17	0.02	12.18
C28+C29tricyclics	0.39	0.34	0.42	0.38	0.04	10.36
27Ts	0.52	0.51	0.49	0.51	0.02	3.17
28ab	0.15	0.12	0.1	0.12	0.02	18.6
25nor30ab	0.07	0.06	0.06	0.06	0.01	9.8
29ab	0.9	0.92	0.88	0.9	0.02	2.01
29Ts	0.16	0.15	0.15	0.15	0.01	6.18
30d	0.05	0.04	0.04	0.05	0.01	14.65
30O	0.09	0.08	0.09	0.09	0	5.72
30G	0.14	0.13	0.13	0.13	0	3.64
29ba	0.07	0.07	0.07	0.07	0	3.47
29aaS	0.87	0.87	1	0.92	0.08	8.41
29bb	0.98	0.93	1.02	0.98	0.05	4.75
27bbSTER	0.75	0.71	0.72	0.73	0.02	2.55
28bbSTER	0.31	0.32	0.32	0.32	0.01	2.52
29bbSTER	0.51	0.52	0.51	0.51	0.01	1.09
TA21	4.86	4.99	4.64	4.83	0.17	3.62
TA26	0.44	0.43	0.44	0.44	0.01	1.18
TA27	1.03	1.06	1.06	1.05	0.02	1.67
2-MP/1-MP	2.14	2.14	2.18	2.16	0.02	1.16
4-MD/1-MD	2.43	2.42	2.49	2.45	0.04	1.44
C2-dbt/C2-phe	0.63	0.63	0.65	0.63	0.02	2.5
C3-dbt/C3-phe	0.8	0.77	0.8	0.79	0.02	2.1
C3-dbt/C3-chr	2.95	2.8	2.53	2.76	0.21	7.6
Retene/C4-phe	0.04	0.05	0.04	0.04	0	6.52
B(a)F/4-Mpy	0.46	0.46	0.45	0.45	0.01	1.95
B(b+c)F/4-Mpy	0.28	0.27	0.27	0.27	0.01	2.2
2Mpy/4-Mpy	0.95	0.97	0.96	0.96	0.01	1.16
1Mpy/4-Mpy	0.93	0.91	0.96	0.94	0.02	2.4

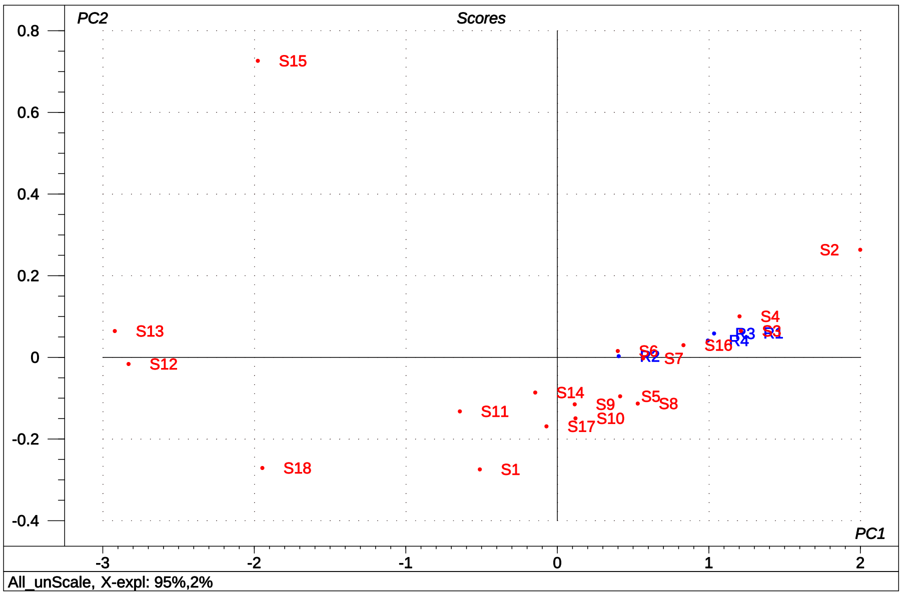

Figure 5.14: PCA score plot performed on all sample data from "MS Server" accident without autoscaling the variables. See Table 5.4 for remark.

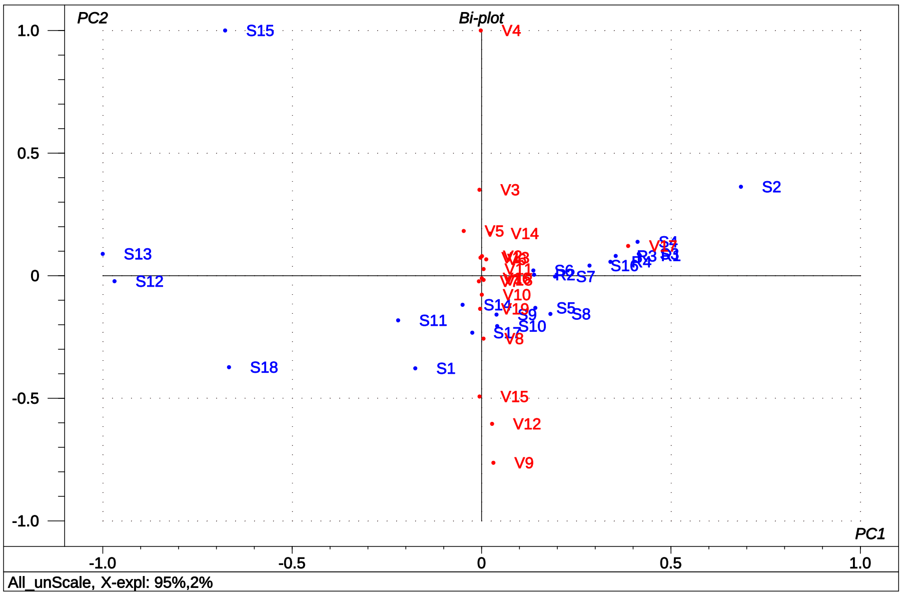

Figure 5.15: PCA biplot performed on all sample data from "MS Server" accident without autoscaling the variables. See Table 5.4 for remark.

Fig.5.16 is the score plot of PCA after removing samples from Gryllefjord, teflon pad sample taken at Fedje, and bird Feather samples taken from Træna, and Lurøy. These figures still show another possible sample that lay far from others, i.e. teflon pad sample from Herdla vest and bird feathers sample from Osnessanden. Hotelling view shown in Fig.5.17 clears up the position of these samples. According to this figure, sample from room 2 and teflon pad sample from Herdla vest are probably not match to any references. Whilst, bird feathers sample from Osnessanden is probably match to the references.

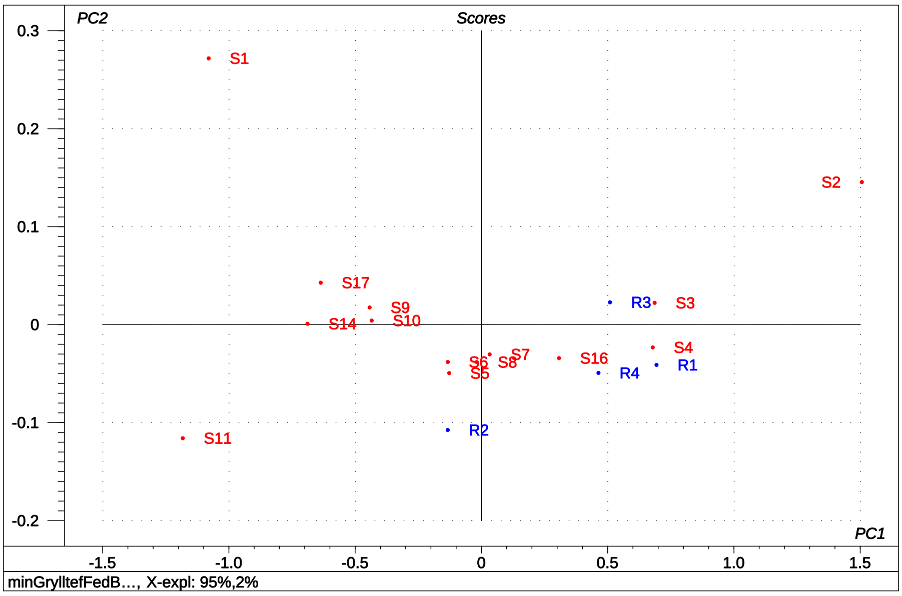

Figure 5.16: PCA score plot performed on data from "MS Server" accident without autoscaling the variables. Samples from Gryllefjord, Teflon pad sample from fedje, birds feathers sample from Tæna, and Lurøy were removed. See Table 5.4 for remark.

As explained in Sect.3.3, there is no clear explanation about oil type of sample taken from room 2. This sample was also not considered as reference sample even though room 2 is part of the ship. More over GC-FID chromatogram of this sample shows different pattern from most of all reference samples and the difference is not cause by weathering. See Table 4.1. This sample could be not match to the references sample and therefore was removed for the next PCA run.

Another possible not match sample is teflon pad sample taken at Herdla vest. The GC-FID chromatogram of this sample shows different pattern with all reference sample. Therefore, this sample was also removed for the next PCA.

PCA score plot after removing the non-match samples in Fig.5.17 is shown in Fig.5.18. This figure indicates that the rest of oil samples are positive match to oil from "MS Server".

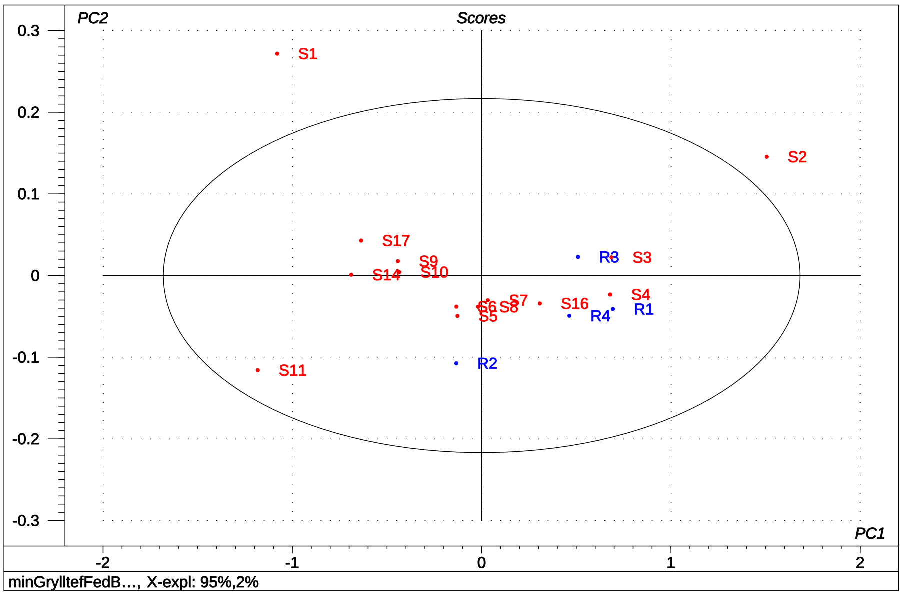

Figure 5.17: PCA Hotteling view performed on data from "MS Server" accident without autoscaling the variables. Samples from Gryllefjord, Teflon pad sample from Fedje, birds feathers sample from Tæna, and Lurøy were removed. See Table 5.4 for remark.

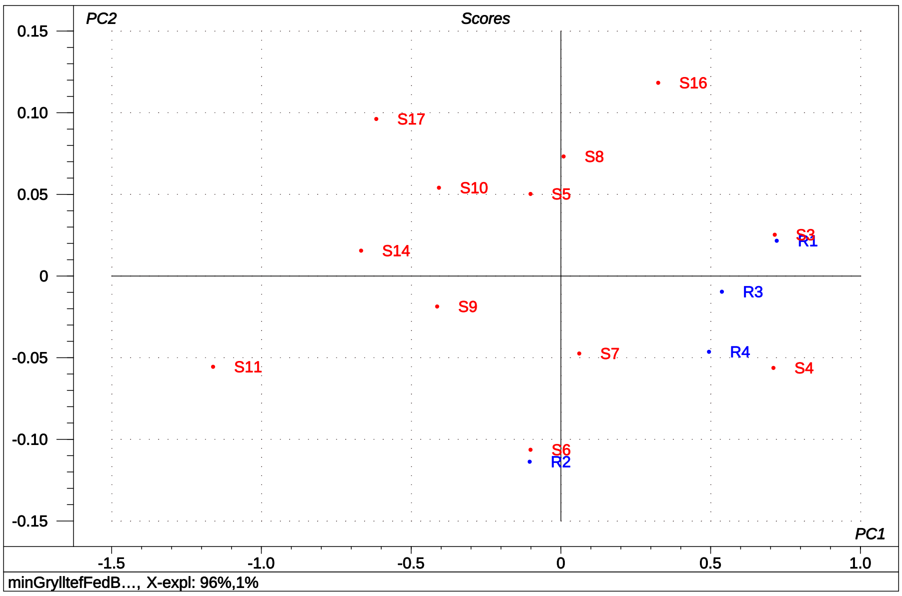

Figure 5.18: PCA score plot performed on data from "MS Server" accident without autoscaling the variables. Samples from Gryllefjord, oil sample from room 2, Teflon pad sample from Fedje and Herdla vest, birds feathers sample from Tæna, and Lurøy were removed. See Table 5.4 for remark.

Table 5.4: Remark explanation for "server" Case

Remark	Sample name	Remark	variable name
R1	Fedje	V1	29bbSTER
R2	rom 3	V2	2Mpy/4-Mpy
R3	rom 4	V3	2-MP/1-MP
R4	KV Eigun	V4	TA26
S1	rom 2	V5	4-MD/1-MD
S2	Teflon Herdla vest	V6	TA27
S3	Kelp Herdla Vest	V7	B(a)F/4-Mpy
S4	Gudbrandsøy	V8	29ab
S5	oil selje	V9	C3-dbt/C3-phe
S6	oil Kvamsøy	V10	B(b+c)F/4-Mpy
S7	oil Stongholmsvikjo	V11	1Mpy/4-Mpy
S8	oil Ivasanden	V12	C2-dbt/C2-phe
S9	Bird gannet	V13	28bbSTER
S10	Bird guillemot	V14	27bbSTER
S11	Bird Osnessanden	V15	27Ts
S12	Birds Lurøy	V16	29ba
S13	birds Træna	V17	TA21
S14	oil Herøy	V18	30G
S15	Oil Gryllefjord	V19	29bb
S16	Oil Vetvika		
S17	Oil Fyrsundet		
S18	teflon Fedje		

5.3.2 *Principal Component Analysis With Autoscaling the Variables*

As in the "MV Full City" oil spill case, some variables to be used in this analysis have different range. For example, variable 30G has value from 0.03-0.05, while variable TA21 ranged from 0.4-4.9. By autoscaling or weighting variables, i.e. by dividing each element in **X**-matrix with its standard deviation, all variables will have the same chance to influence the model. Fig.5.19-5.27 show the result of PCA performed on the DRs data of "MS Server" oil spill identification.

If all samples were included, score plot of PCA (autoscaled variable) as presented in Fig.5.19 shows some samples that not match to references samples. These samples are identical to the one for without autoscaled variables explained in Sect.5.3.1. Removing these samples, the score plot is then shown in Fig.5.20.

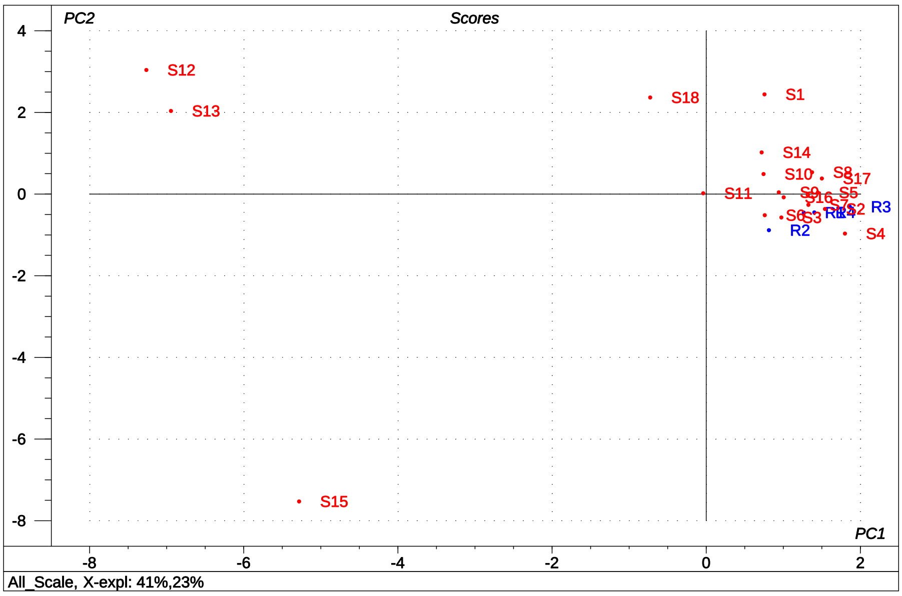

Figure 5.19: PCA score plot for "Server" oil spill identification. All variables are scaled by 1/STD. See Table 5.4 for remark.

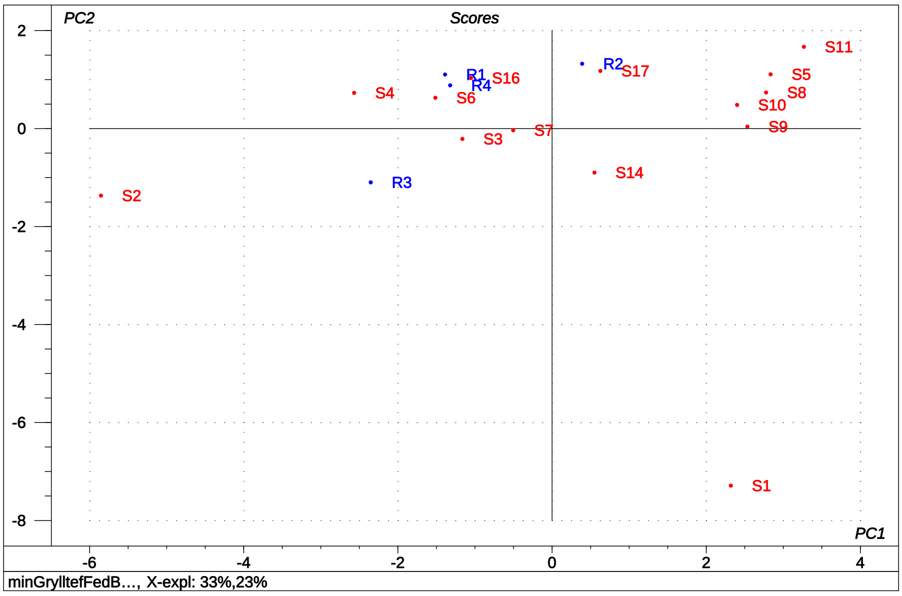

Figure 5.20: PCA Score plot of data from "Server"accident after removing sample from Gryllefjord, Teflon pad sample from fedje, birds feathers sample from Tæna, and Lurøy. All variables are scaled by 1/STD. See Table 5.4 for remark.

Again, Fig.5.20 shows another possible not match samples. Fig.5.21 confirmed that these not match samples are the ones from room 2 and teflon pad sample taken at Herdla vest.

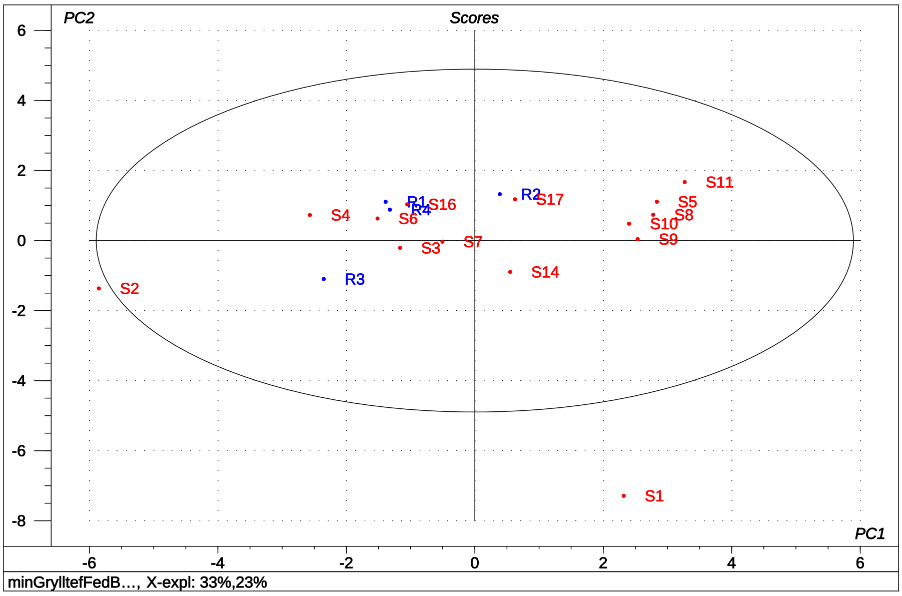

Figure 5.21: PCA Hotteling view of data from "Server" accident after removing sample from Gryllefjord, room 2, teflon pad sample from fedje and Herdla vest, birds feathers sample from Tæna, and Lurøy. All variables are scaled by 1/STD. See Table 5.4 for remark.

PCA score plot after removing sample from room 2 and teflon pad sample taken at Herdla vest is presented in Fig.5.22. Hotelling view of this PCA presented in Fig.5.23 shows another not match sample, i.e sample from Fyrsundet. This is different if we compare to the one without autoscaled the variables as explained in Sect.5.3.1. This differences are because all variable have the same chance to influence the model, whilst the one without autoscaling the variable, the higher value of of a variable the higher its influence to the model. This seems strange since its location closed to Fedje, casualty area, but the sampling time which is six months after casualty could explain this phenomena. This sample may have been very weathered so that almost all of the component of the oil is changed. Another possibility is that it does not belong to oil from "MS Server" casualty. Other classification method such as cluster analysis or PLS-DA will be useful to define this sample.

The next PCA run was done without sample from Fyrsundet. Score plot of this PCA presented in Fig.5.24 shows another possible not match sample. This sample was taken on 25th April 2007 at Vetvika, Bremanger municipality. This sampling date explains why this sample may be not match to the reference. Removing this sample for the next PCA run, the score plot is then shown in Fig.5.25.

No more sample is detected as not match in this PCA run. This is confirmed by Hotelling view in Fig.5.26. This means, the samples are positive match to the "MS Server" oil. The samples seems to be divided into two clusters. The

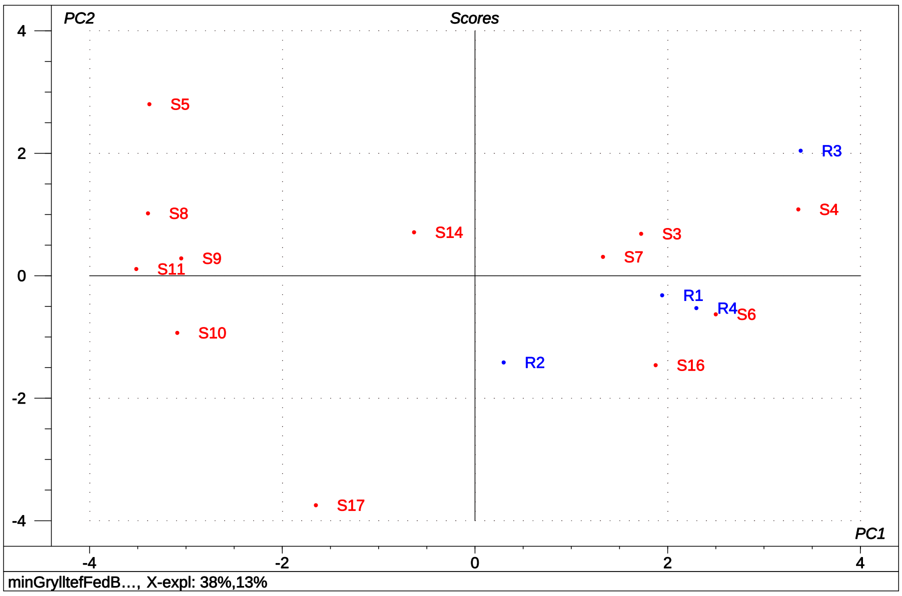

Figure 5.22: PCA score plot of data from "MS Server" accident after removing sample from Gryllefjord, room2, teflon pad sample from Fedje and Herdla vest, birds feathers sample from Tæna, and Lurøy. All variables are scaled by 1/STD. See Table 5.4 for remark.

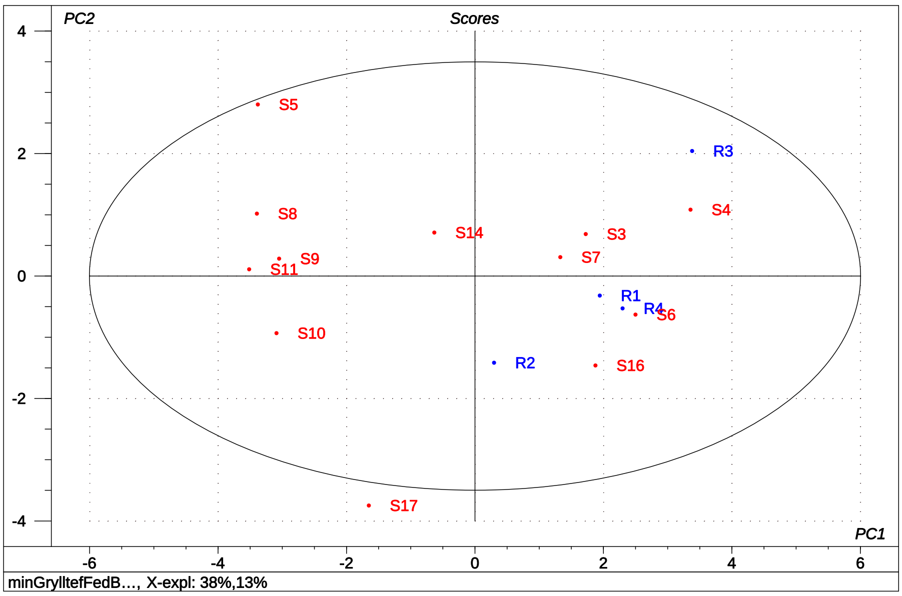

Figure 5.23: PCA Hotelling view of data from "MS Server" accident after removing sample from Gryllefjord, room2, teflon pad sample from fedje and Herdla vest, birds feathers sample from Tæna, and Lurøy. All variables are scaled by 1/STD. See Table 5.4 for remark.

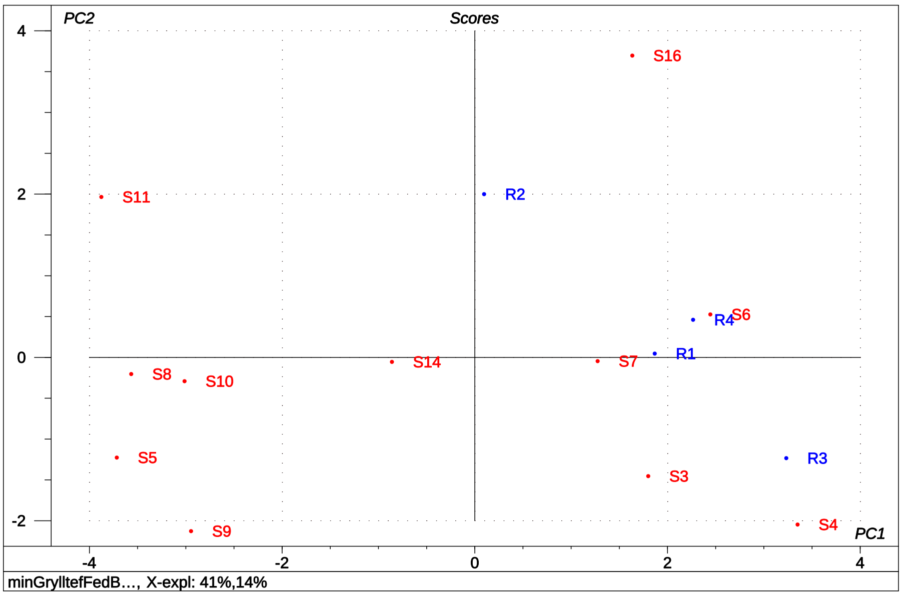

Figure 5.24: PCA score plot of data from "MS Server" accident after removing sample from Gryllefjord, room2, Fyrsundet, teflon pad sample from fedje and Herdla vest, birds feathers sample from Tæna, and Lurøy. All variables are scaled by 1/STD. See Table 5.4 for remark.

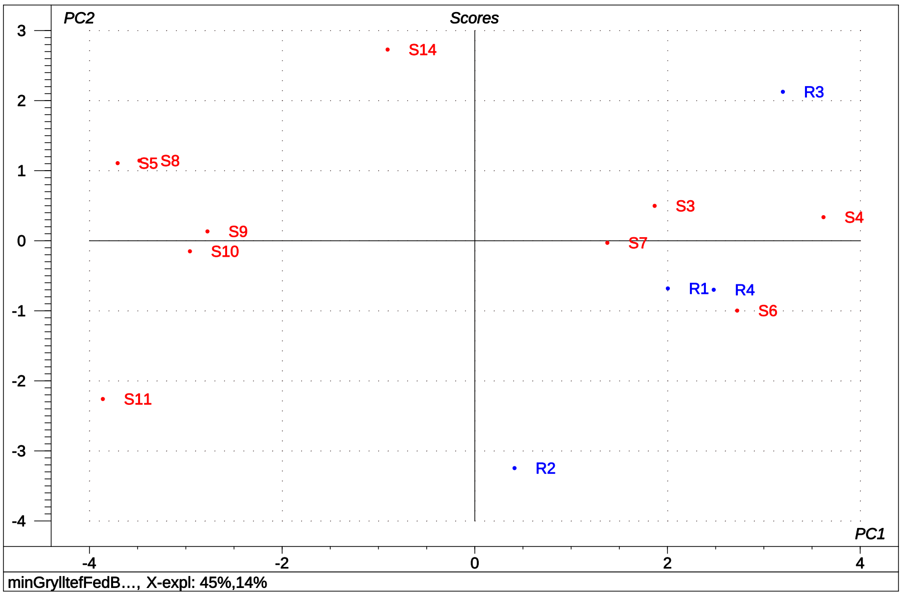

Figure 5.25: PCA score plot of data from "MS Server" accident without sample from Gryllefjord, room2, Fyrsundet, Vetvika, teflon pad sample from fedje and Herdla vest, birds feathers sample from Tæna, and Lurøy. All variables are scaled by 1/STD. See Table 5.4 for remark.

first cluster (on the positive direction of PC1) contains reference samples, spill sample from Kvamsøy, Gudbrandsøy, Stongholmvika, and Kelp sample from Herdla vest. The second cluster contain some bird feather samples and oil sample from Herøy, Ivasanden and Selje kommune.

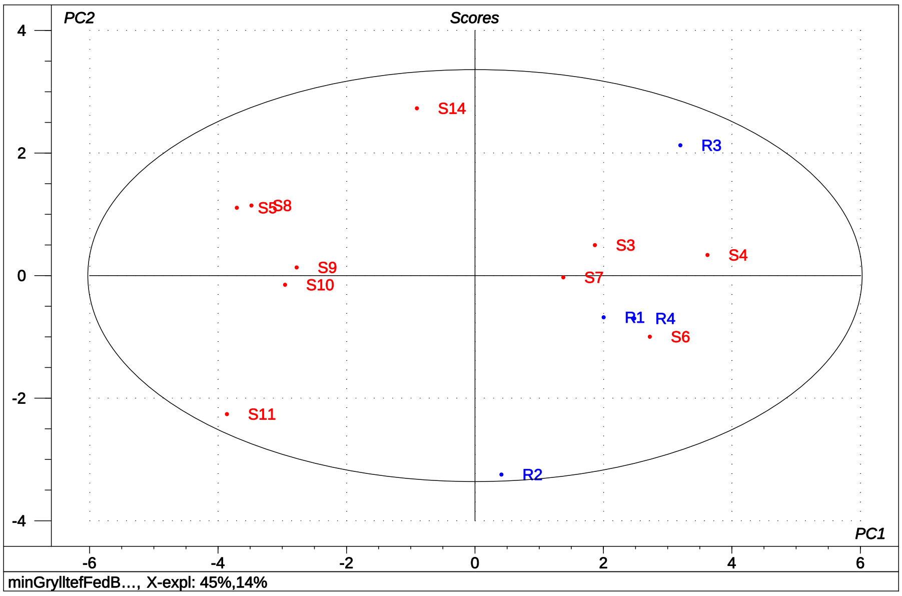

Figure 5.26: PCA Hotelling view of data from "MS Server" accident without sample from Gryllefjord, room2, Fyrsundet, Vetvika, teflon pad sample from fedje and Herdla vest, birds feathers sample from Tæna, and Lurøy. All variables are scaled by 1/STD. See Table 5.4 for remark.

The second cluster seems to be more subjected by weathering processes. This can be explained by looking at the date and the sampling location. All samples in the second cluster were taken $4-19$ days after the accident. The sampling location ranges from $105-205$ km. Whilst, some samples in the first cluster, i.e sample from Stongholmsvikjo, Gullbrandsøy, could not be easily explained by looking at the sampling location since the author could not find the exact position of this area in the map. Sample from Kvamsøy which is taken for 21 days after casualty and located at approximately 200 km also part of the first cluster. This needs another analysis to explain this phenomena.

Loading plot in Fig.5.27 shows the variables which were highly affected by the first cluster are 27bbSTER and 30G. Whilst, the second cluster was highly affected by variable 29bbSTER and C3-dbt/C3-Phe.

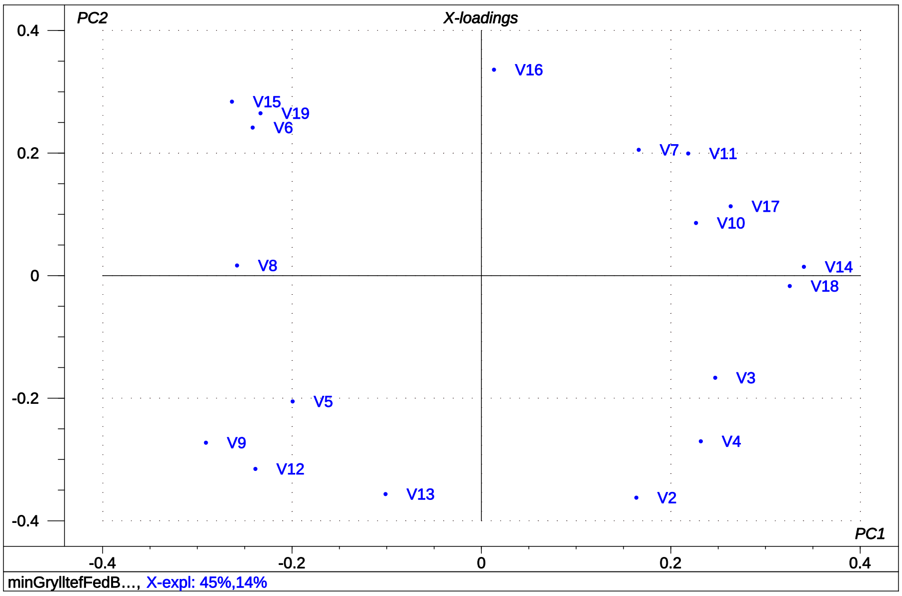

Figure 5.27: PCA loading plot of data from "MS Server" accident without sample from Gryllefjord, room2, Fyrsundet, Vetvika, teflon pad sample from fedje and Herdla vest, birds feathers sample from Tæna, and Lurøy. All variables are scaled by 1/STD. See Table 5.4 for remark.

6 HIERARCHICAL CLUSTER ANALYSIS

6.1 GENERAL

The previous chapter presents classification based on visual inspection of score plot using PCA. Sometimes a cluster can be distinguished based on their size, circular, spherical, elongated or curved arrangements of the objects. More often, this classification is difficult because the objects form clusters with different shapes and densities [Bratchell, 1992]. The latter seemed to be occurred when the author performing PCA for oil spill identification in this work. The simplest way for cluster analyses are based on the measurement of distance or similarity of objects. Selection of the distance or similarity is based on the type of variable to be used in the analysis (see Sect.2.4.4).

As presented in this chapter, cluster analysis was performed using hierarchical methods because of its simplicity, rapid to compute, give straightforward and intuitive interpretation [Bratchell, 1992]. Three types of linkage, i.e. single linkage, average linkage and furthest neighbor, were used for comparison. Once again, *MATLAB* was used to perform the method. The results are presented in dendrograms.

Cluster analysis was applied to the score value data from the last PCA run of each spill case. Only score value of PC 1 until optimal PC number were used for the analysis. This was to avoid participation of sample outliers in the classification. The variables were continuous variables, therefore the most suitable distance to be used for clustering was euclidean distance [Bratchell, 1992].

6.2 HIERARCHICAL CLUSTER ANALYSIS OF "FULL CITY"OIL SPILL CASE

6.2.1 *Hierarchical Cluster Analysis Applied to Unscaled Principal Component Analysis*

Fig.6.2 was used to find optimal PC number obtained from the last PCA in Sect.5.2.1. The plot reaches its plateau in PC 8. PC 4 was chosen as optimum PC number. Score value from PC1 until PC 4 is given in Table 6.2 for unscaled PCA and Table 6.3 for autoscaled PCA.

Fig.6.3-6.5 show the results of cluster analysis using Euclidean distance for single linkage, average linkage and furthest neighbor linkage, respectively. The figures show dendrograms (using furthest neighbor), which perform the clearest classification. This is because the samples naturally tend to form different clusters. Whilst, single linkage or average linkage are more appropriate for samples that tend to form "chain like" cluster type [Statsoft, 2011].

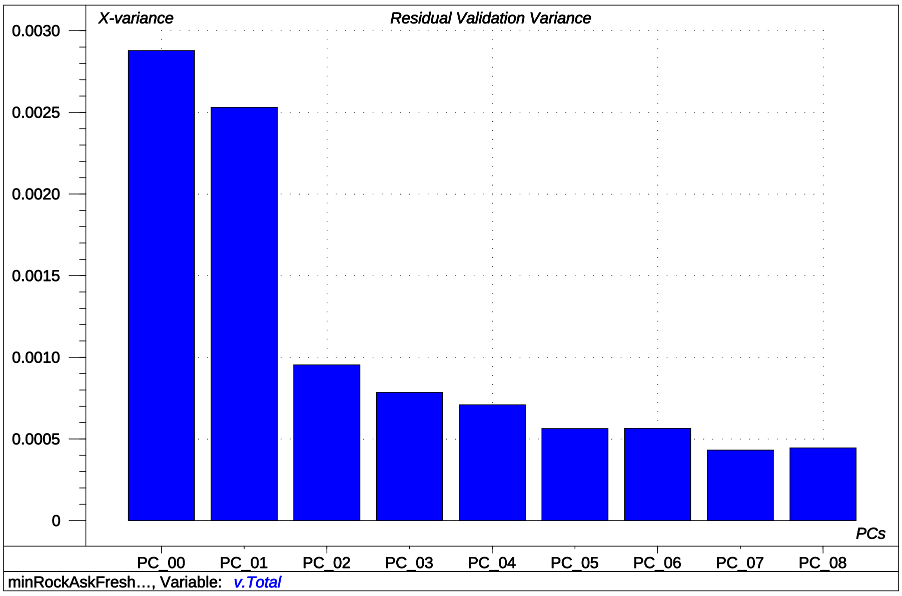

Figure 6.2: Residual variance plot obtained from final PCA run of "Full City" accident. No variables were scaled.

Table 6.2: Score value of unscaled PCA applied to "Full City" Case

Samples	PC_01	PC_02	PC_03	PC_04
Krogshavn 3107 ref	-0.36	-0.10	0.01	0.02
Oddane 3107	0.15	0.05	-0.01	0.07
Mandal 0308	0.05	0.08	0.06	0.02
Nevlunghavn 0608	-0.08	-0.06	-0.04	0.05
Langesund bad 0708	-0.12	0.26	-0.09	-0.03
Grimstad 0208	0.09	-0.15	-0.03	-0.01
Risor 0108	0.15	0.03	0.00	0.01
Arendal 0708	0.08	-0.19	-0.04	-0.05
Lillesand 1908	0.10	0.05	0.02	-0.05
Såstein	-0.07	0.02	0.14	-0.02

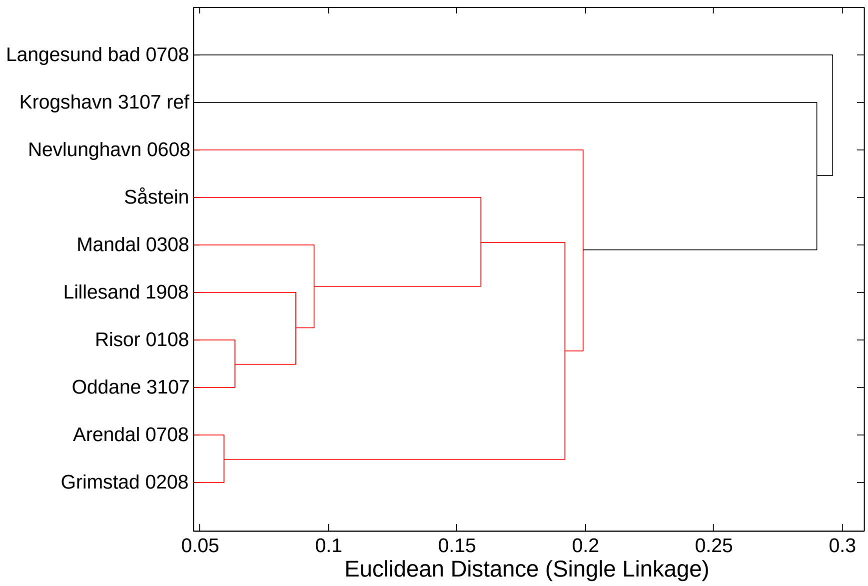

Figure 6.3: Single linkage Euclidean distance dendrogram of "Full City" case. No variables were scaled.

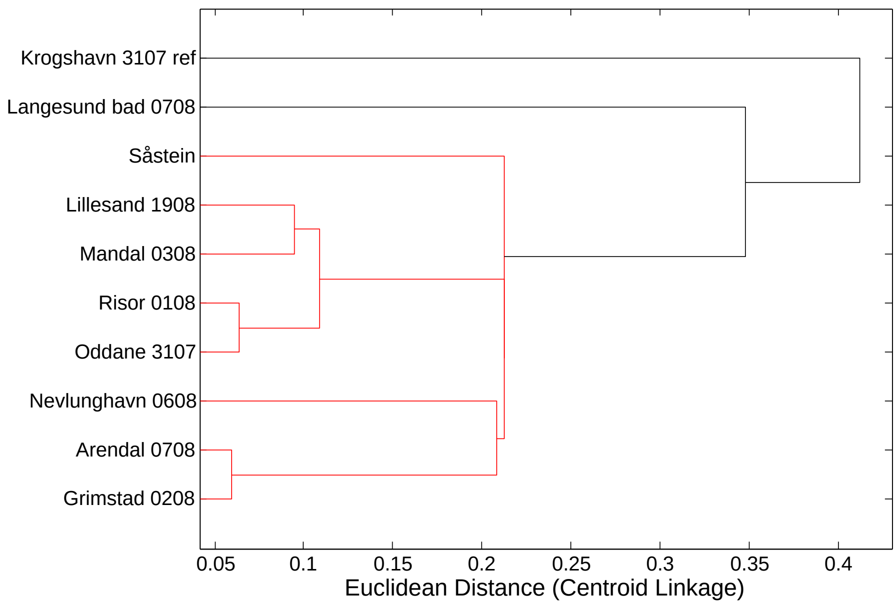

Figure 6.4: Average linkage Euclidean distance dendrogram of "Full City" case. No variables were scaled.

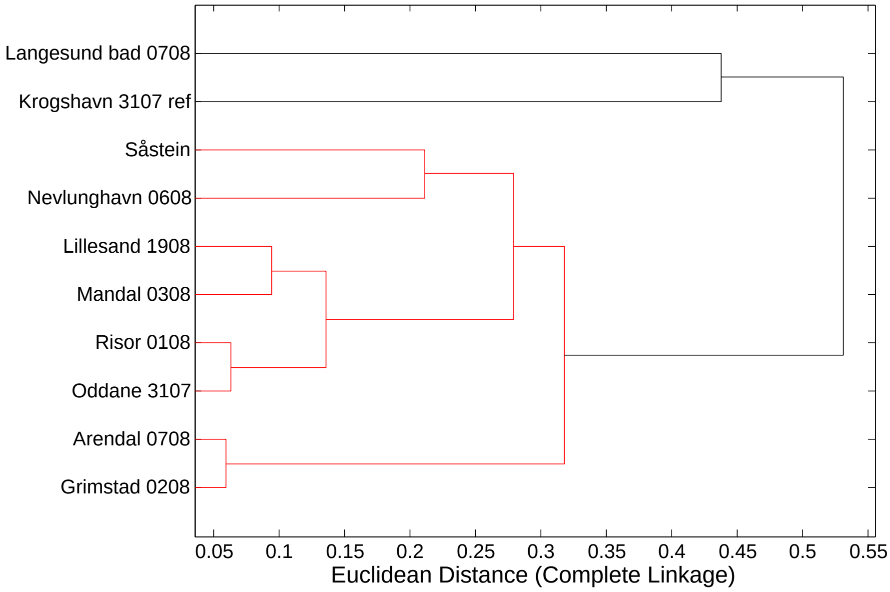

Figure 6.5: Complete linkage Euclidean distance dendrogram of "Full City" case. No variables were scaled.

Fig.6.5 shows two main clusters. Sample taken from Såstein is clustered together with sample from Nevlunghavn, Lillesand, Mandal, Risor, Oddane, Arendal, and Grimstad. Whilst, sample from Krogshavn is clustered together with sample from Langesund bad. This classification is similar as performed by Faksness et al. [2010], which applied CEN-method. The dendrogram also shows greatest similarity of sample from Nevlunghavn with sample from Såstein. This meets the conclusion given by Faksness et al. [2010].

6.2.2 *Cluster Analysis Applied to Autoscaled Principal Component Analysis*

Fig.6.6 was used to find optimal PC number obtained from the last PCA in Sect.5.2.1. The plot reaches its plateau in PC 9. And consecutively PC 6 was chosen as optimum PC number. Therefore, score values of PC1-PC6 were used for clustering. Fig.6.7-6.8 show the results of cluster analysis using euclidean distance for single linkage, average linkage, and furthest neighbor (or complete) linkage, respectively.

As in Sect.6.2.1, dendrogram using complete linkage shows the clearest separation among clusters. This dendrogram is presented in Fig.6.9. The dendrogram shows the same tendency as performed using the unscaled PCA score. Sample taken from Såstein is clustered together with sample from Nevlunghavn, Lillesand, Mandal, Risor, Oddane, Arendal, and Grimstad. Whilst, sample from Krogshavn is clustered together with sample from Langesund bad. The dendrogram also shows greatest similarity of sample from Nevlunghavn with sample from Såstein. This meets the conclusion given by Faksness et al. [2010] using CEN-method.

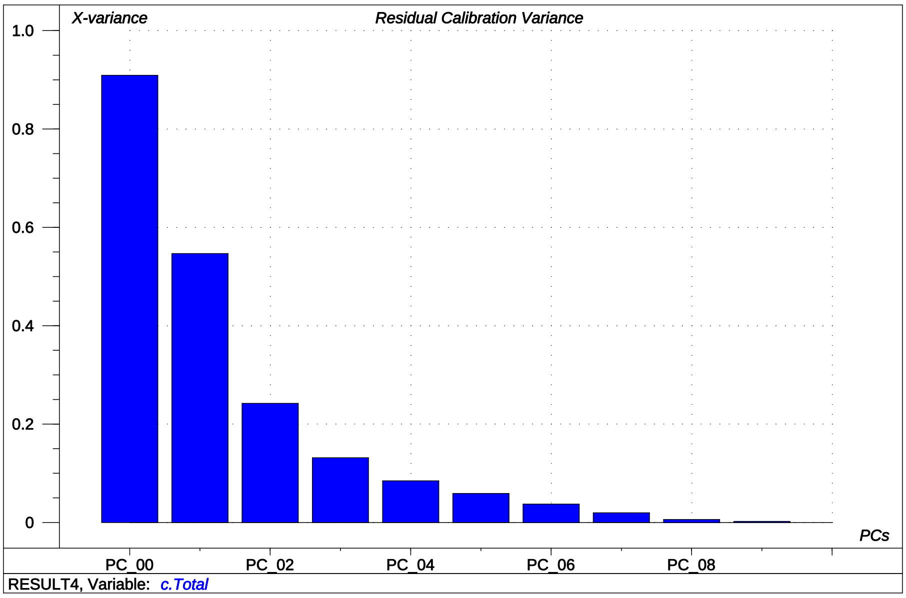

Figure 6.6: Residual variance plot obtained from Final PCA run of "Full City" accident. All variables were scaled by 1/STD.

Table 6.3: Score value of scaled PCA applied to "Full City" Case

Sample	PC_01	PC_02	PC_03	PC_04	PC_05	PC_06
Krogshavn 3107 ref	6.682	-1.424	1.149	0.471	0.139	-0.257
Oddane 3107	-3.149	1.595	3.087	0.321	0.391	-0.124
Mandal 0308	-1.036	-0.372	-0.006	-1.559	-1.285	0.950
Nevlunghavn 0608	0.937	-1.462	-0.156	-0.200	-1.097	-1.194
Langesund bad 0708	4.511	3.905	-0.921	0.110	-0.069	0.361
Grimstad 0208	-1.485	-1.524	-0.018	0.837	-0.798	0.488
Risor 0108	-3.114	1.298	-1.166	-0.226	0.137	-1.475
Arendal 0708	-1.717	-0.957	-1.200	1.999	0.572	0.492
Lillesand 1908	-2.044	0.616	-0.382	-0.259	0.123	0.624
Såstein	0.414	-1.674	-0.387	-1.493	1.888	0.134

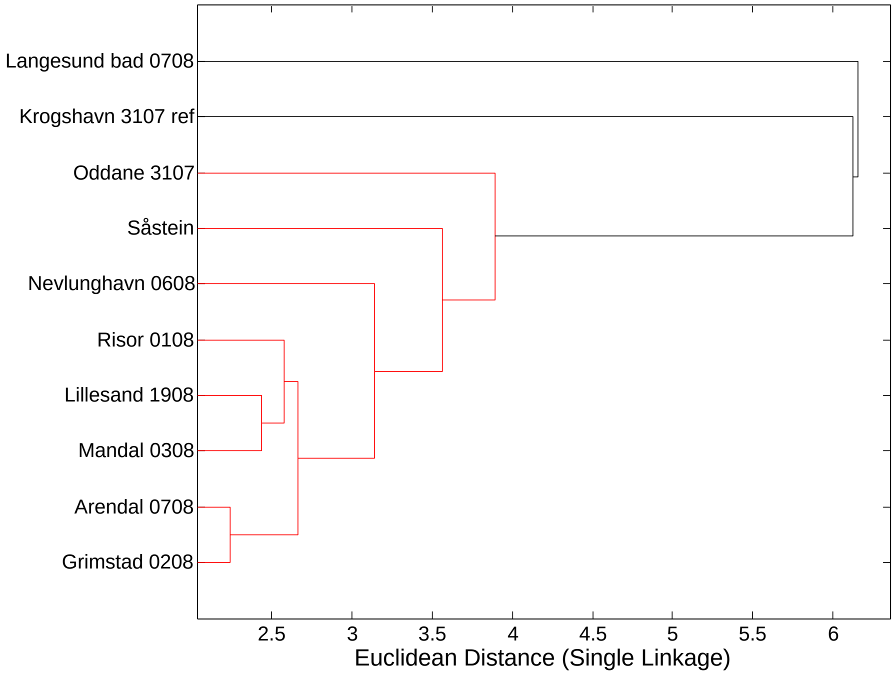

Figure 6.7: Single linkage Euclidean distance dendrogram of "Full City" case. All variables were scaled by 1/STD.

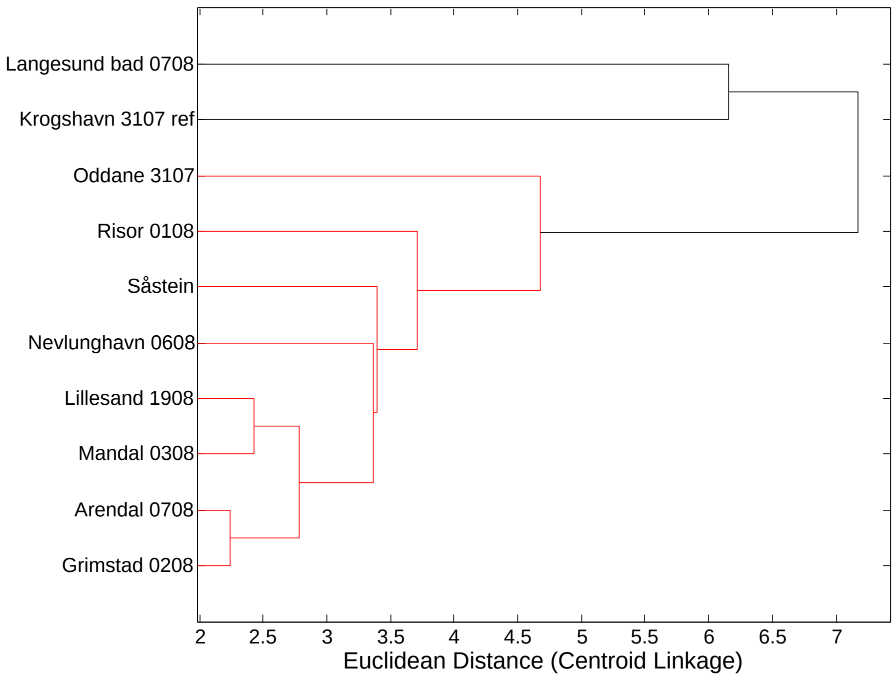

Figure 6.8: Average linkage Euclidean distance dendrogram of "Full City" case. All variables were scaled by 1/STD.

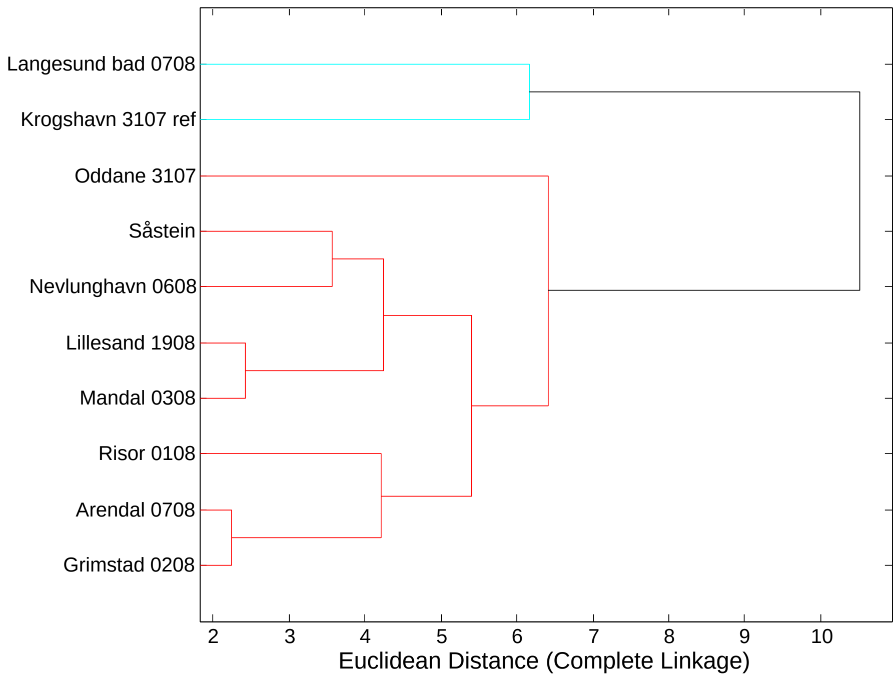

Figure 6.9: Complete linkage Euclidean distance dendrogram of "Full City" case. All variables were scaled by 1/STD.

6.3 cluster analysis of "server"oil spill case

6.3.1 *Cluster Analysis Applied to Unscaled Principal Component Analysis*

Fig.6.10 was used to find optimal PC number obtained from the last PCA in Sect.5.2.1. The plot reaches its plateau in PC 14. PC 3 was chosen as optimum PC number. Score values of these PC were shown in Table 6.4.

The dendrograms of this hierarchical cluster analysis are shown in Fig.6.11 - 6.13. Again, dendrogram which was developed using furthest linkage, as presented in Fig.6.12, shows the clearest separation between clusters. The samples are clustered into two main clusters. First, cluster (blue line) representing samples which are very similar to the reference samples (samples taken from Herdla Vest and Gudbrandsøy). This similarity was because they were taken not far from the accident area and were taken soon after accident.

The second cluster represents samples, which are more weathered. These samples were taken quite far (at least 100 km) from the accident area and most of them (especially bird feathers samples) were taken two weeks after the casualty (see Table 3.3 and 3.4).

6.3.2 *Cluster Analysis Applied to Autoscaled Principal Component Analysis*

Fig.6.14 was used to find optimal PC number obtained from the last PCA in Sect.5.2.1. The plot reaches its plateau in PC 12. PC 6 was chosen as optimum PC number. The score value of these PCs was presented in Table 6.5.

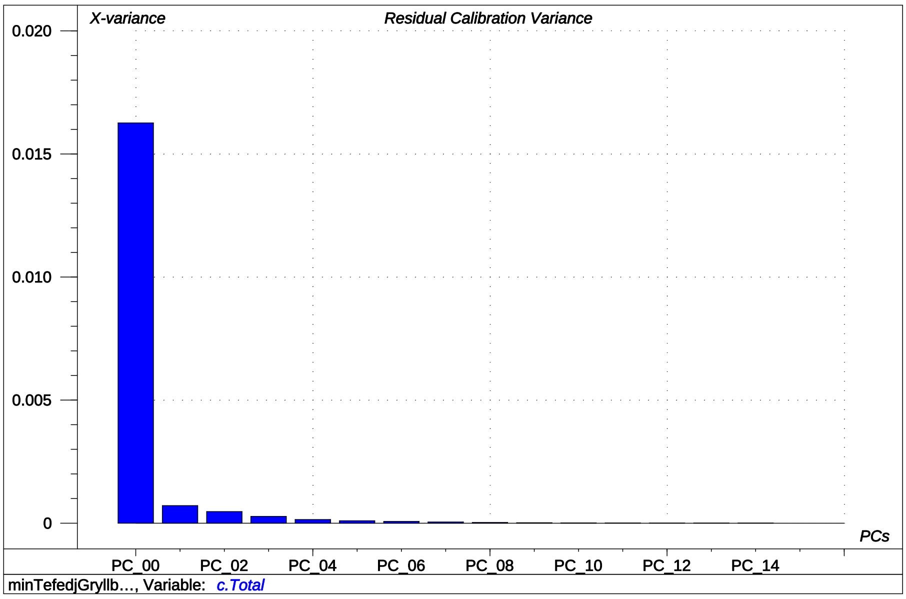

Figure 6.10: Residual variance plot obtained from final PCA run of "Server" accident. No variables were scaled.

Table 6.4: Score value of unscaled PCA applied to "Server" Case

Samples	PC_01	PC_02	PC_03
Fedje Ref	0.63	-0.05	0.03
Rom3	-0.20	-0.10	-0.08
rom4	0.45	-0.02	-0.04
KV eigun	0.40	-0.10	0.00
Teflon Herdla vest	1.45	0.20	-0.03
Kelp Herdla Vest	0.63	-0.03	0.02
Gudbrandsøy	0.62	-0.10	-0.02
oil selje	-0.20	-0.01	0.12
oil Kvamøy	-0.20	-0.08	-0.09
oil Stongholmsvikjo	-0.03	-0.05	-0.03
oil Ivasanden	-0.08	-0.02	0.13
Bird gannet	-0.51	-0.02	0.05
Bird guillemot	-0.50	0.02	0.08
Bird Osnessanden	-1.25	0.03	-0.06
oil Herøy	-0.75	0.08	-0.04
Oil Vetvika	0.24	0.10	-0.03
Oil Fyrsundet	-0.70	0.14	-0.01

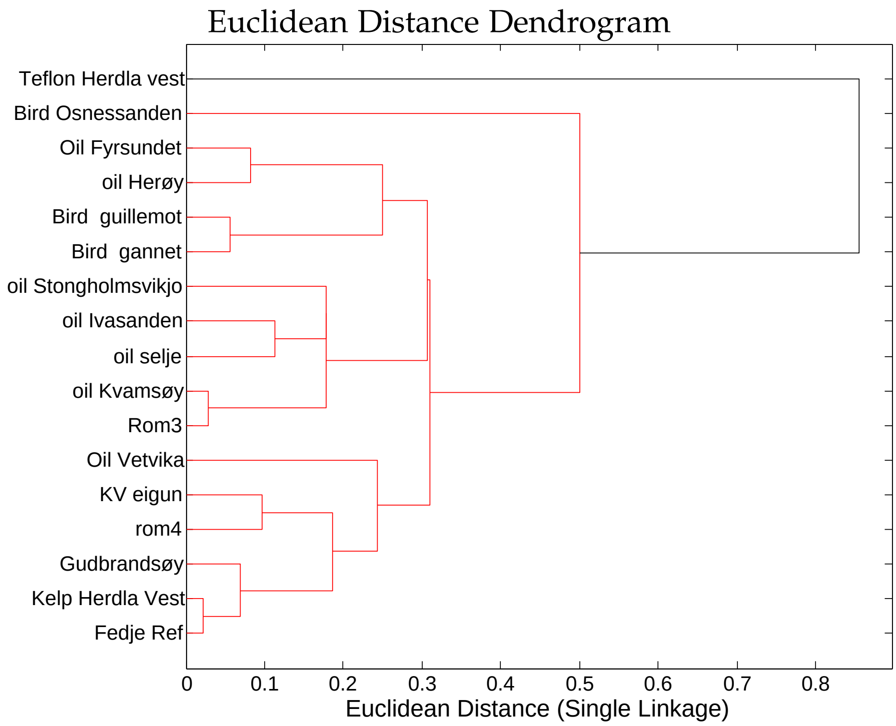

Figure 6.11: Single linkage Euclidean distance dendrogram of "Server" Case. No variables were scaled.

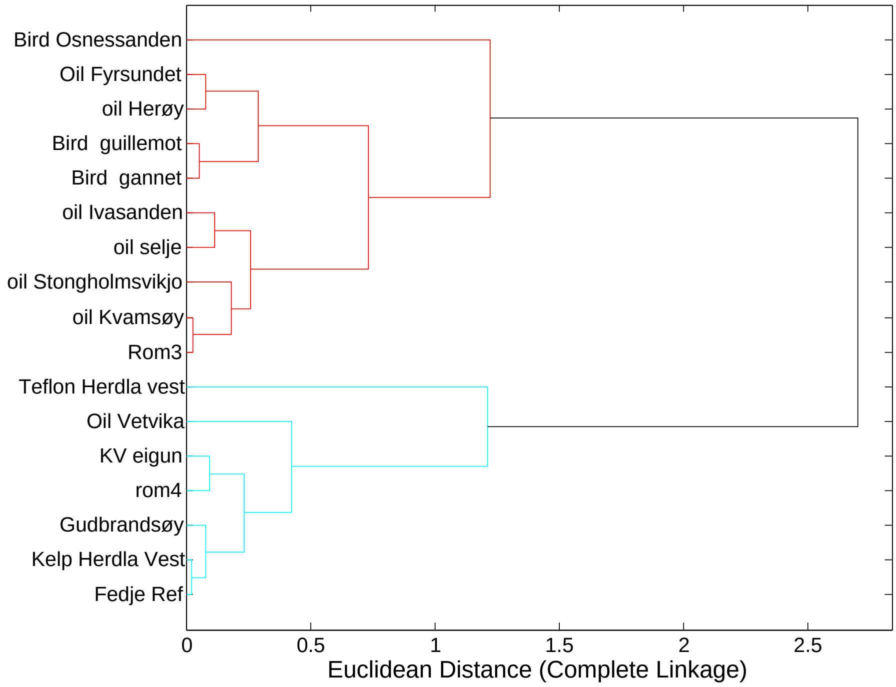

Figure 6.12: Complete linkage Euclidean distance dendrogram of "Server" Case. No variables were scaled.

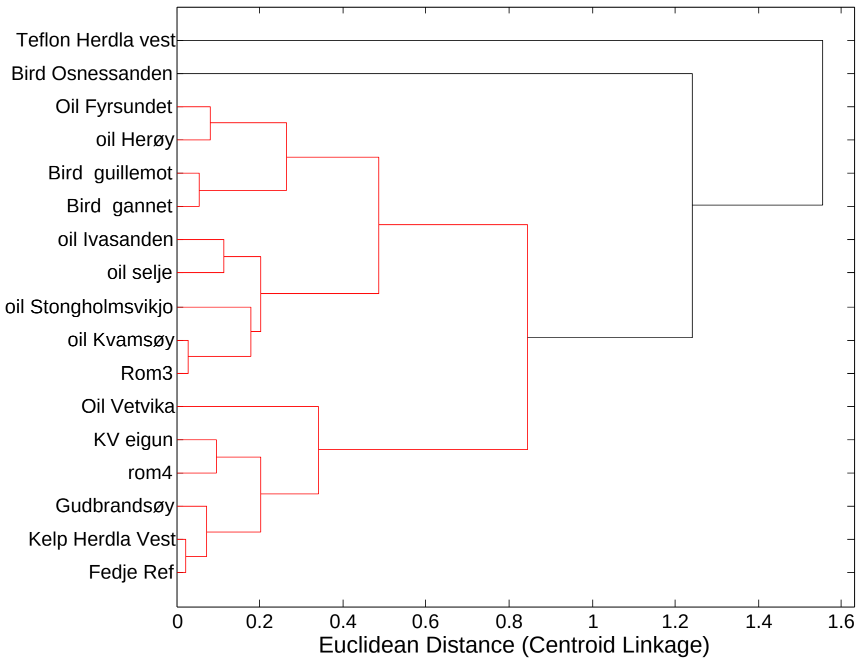

Figure 6.13: Centroid linkage Euclidean distance dendrogram of "Server" Case. No variables were scaled.

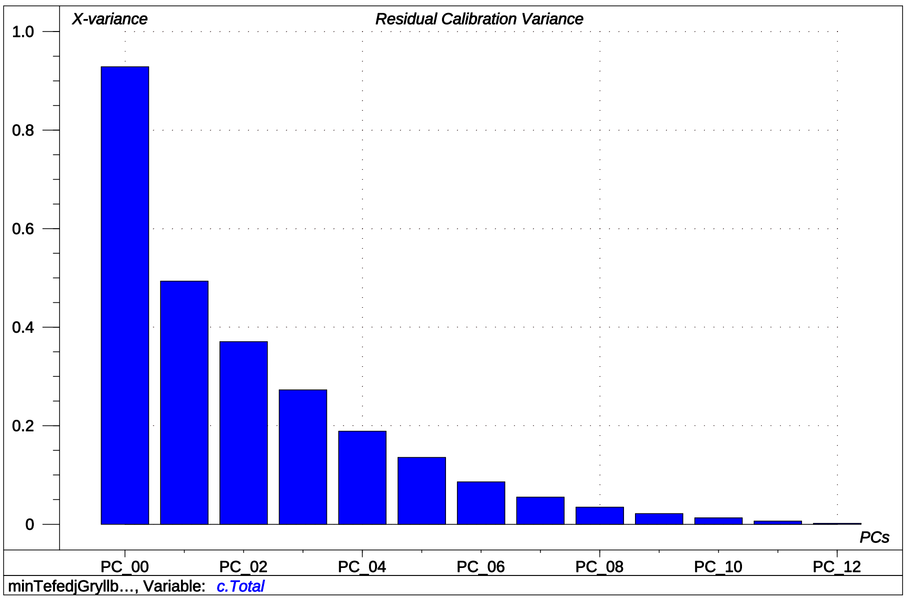

Figure 6.14: Residual variance plot obtained from final PCA run of "MS Server" accident. All variables were scaled by 1/STD.

Table 6.5: Score value of scaled PCA applied to "MS Server" Case

	PC_01	PC_02	PC_03	PC_04	PC_05	PC_06
Fedje Ref	2.02	-0.63	-0.33	0.02	-0.82	-0.73
Rom3	0.68	-3.29	1.11	0.35	1.25	-0.05
rom4	3.41	2.13	-0.51	1.49	1.38	1.10
KV eigun	2.54	-0.65	0.67	-0.25	-0.02	-1.27
Kelp Herdla Vest	2.09	0.48	-1.04	-1.10	0.09	1.32
Gudbrandsøy	3.78	0.39	-1.84	-0.20	-1.00	-0.69
oil selje	-4.09	1.12	-2.25	2.14	-0.46	-0.89
oil Kvamsøy	2.71	-0.91	0.96	-0.04	-1.47	-0.36
oil Stongholmsvikjo	1.59	-0.06	0.33	0.25	1.54	0.45
oil Ivasanden	-3.50	1.05	0.85	-0.23	1.50	-1.84
Bird gannet	-2.90	0.09	-1.40	-2.37	0.15	0.81
Bird guillemot	-3.20	-0.16	0.07	-2.17	-0.18	0.08
Bird Osnessanden	-3.98	-2.30	0.10	1.91	-0.80	1.43
oil Herøy	-1.13	2.76	3.28	0.19	-1.15	0.63

The dendrograms of this hierarchical cluster analysis are shown in Fig.6.15 - 6.17. Once again, dendrogram which was developed using complete linkage,

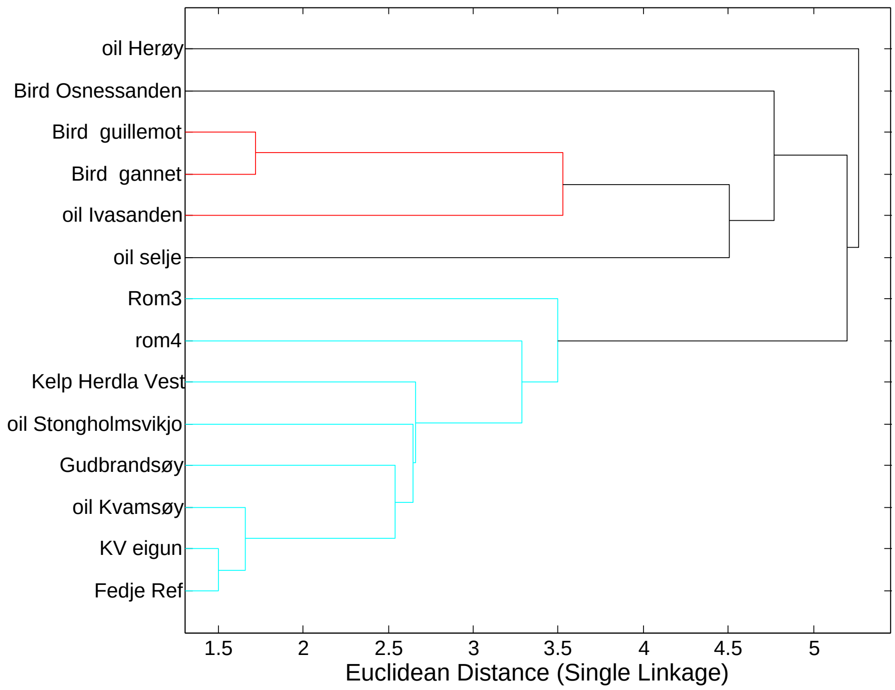

Figure 6.15: Single linkage-Euclidean distance dendrogram of "Server" Case. All variables were scaled by 1/STD.

as shown Fig.6.16, demonstrates clearer explanation as compared to the two

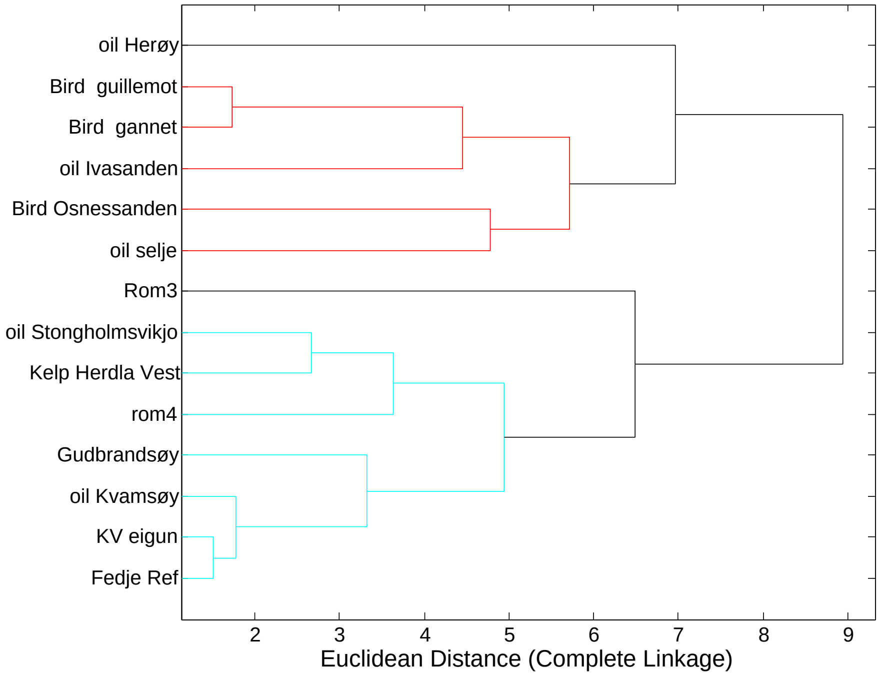

Figure 6.16: Complete linkage-Euclidean distance dendrogram of "Server" Case. All variables were scaled by 1/STD.

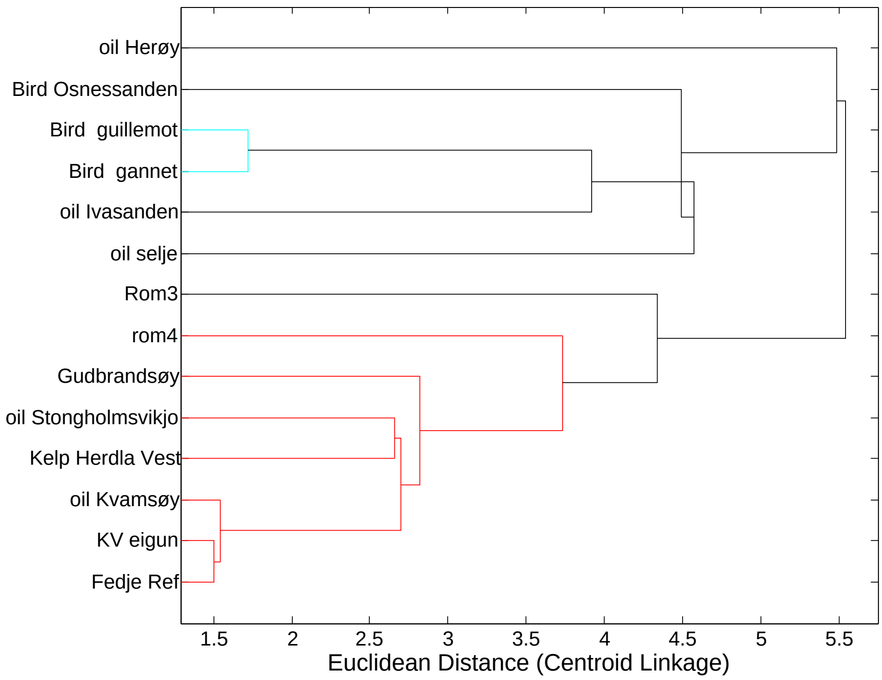

Figure 6.17: Centroid linkage-Euclidean distance dendrogram of "Server" Case. All variables were scaled by 1/STD.

others. This figure classifies the samples into two clusters. The member of the cluster is different as compared to the one using PCA unscaled scores. This is because oil sample from Vetvika and Fyrsundet categorized as non match to "MS Server" by this scaled PCA. Whilst, unscaled PCA categorized them as match to "MS Server" oil.

Fig.6.16 shows oil from Herdla Vest, Selje, Gudbrandsøy and Kvamsøy in the same cluster with the reference samples. Except for sample from Kvamsøy, the similarity in this cluster can be explained by the time they were taken.

The second cluster in Fig.6.16 represents samples that more affected by weathering processes. This cluster consists of samples that were taken quite far (at least 100 km) from the accident area. Again, most of them (especially bird feathers samples) were taken two weeks after accident (see Table 3.3 and 3.4).

7 PARTIAL LEAST SQUARE DISCRIMINANT ANALYSIS

In Chapter 5, PCA was performed to discover whether an oil spill sample matches to the references or not. Data evaluation was performed by visual inspection of its score plot. However, this visual inspection was sometime difficult to be performed because of the shape and the arrangement of the objects. The objectivity of visual interpretation of score plot of PCA can be improved by, e.g. numerical comparisons or statistical comparisons. Many studies showed that either numerical comparison or statistical comparison needs replicated samples so that can give more objective result [Faksness et al., 2002; Christensen and Tomasi, 2007]. This mean more cost will be implied.

Another method that useful for classification is PLS-DA. This method is supervised classification method based on PLS, where class information is stored in **Y** matrix. This method assumes that a sample has to be a member of one of the classes included in the analysis using binary discriminant variable. Here, the discriminant variable is coded by $1 =$ member and $0 =$ not member [CAMO, 2006]. This is useful to classify whether an spill oil match or not to the references.

In this thesis, PLS was performed using *Unscrambler*. PLS2 was used for the analysis since **Y** variable to be used in each oil spill case contain two columns, i.e. one column for "MV Full City" class and one column for "MS Server" class. Due to small amount of samples, cross validation was conducted to the variables. Even though this validation can be used for classification model using small number of sample, this validation only gives a reliable result when proper procedure is performed. In the proper cross validation procedure, the total data should be divided into a training set, a validation set and a test set [Westerhuis et al., 2008]. This cannot be applied for both oil spill cases, which were investigated in this master thesis, because the number of sample is very small. Consequently, such separation into training set, validation set, and test set is not possible. For example, in the "MV Full City" case, the number of sample is 20 and it consists of 3 reference samples. This means that only 3 samples that can be used as training samples. Therefore, PLS-DA was performed by combining the data sets of "MV Full City" and "MS Server" oil spill. This approach enabled the prediction step in PLS-DA. In this case, it is assumed that "MV Full City" accident and "MS Server" accident were happened at the same time.

In this case, the X-variables (diagnostic ratio) of "MV Full City" and "MS Server" to be used for the analysis should be the same. Therefore, variables 30d, 29aaS, C3-dbt/C3-Chr and 29 Ts from "MV Full City" data sets were removed because they are not used in the "MS Server" data sets. Whilst, from "MS Server" data sets, variable C2-dbt/C2-Phe, 29ba, TA21 and 30G were removed. Totally, only 15 variable were employed for the analysis. The Y-variables are variable "FC", which is a representation of oil from "MV Full City", and "Ser", which is a representation of oil from "MS Server". All variables are scaled by 1/STD.

The first step of this method was modeling, which then consecutively followed by prediction step. In modeling step, reference samples from both "MV Full City" and "MS Server" oil spill accidents were utilized. The result is shown in Fig.7.2-7.5.

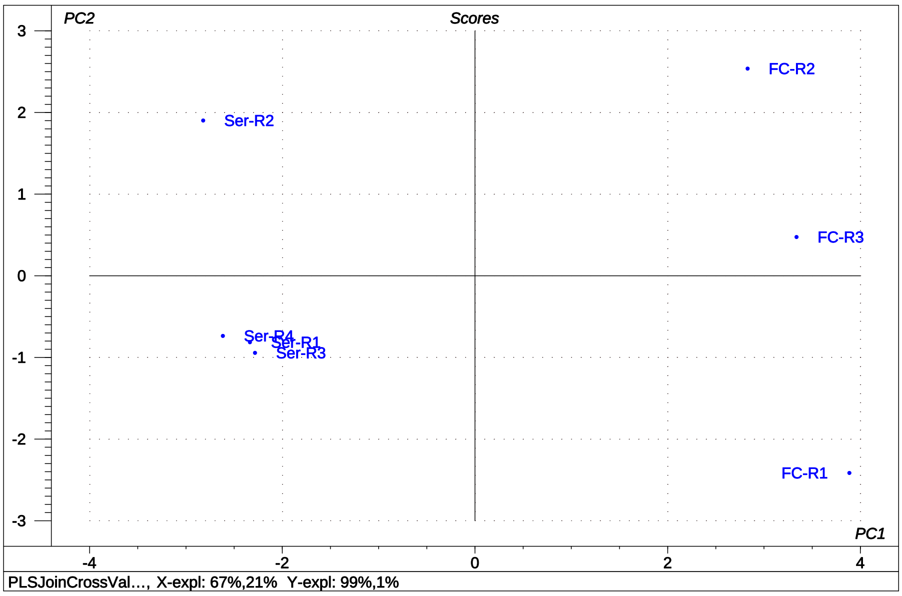

Figure 7.2: Score plot PLS conducted to combined data from "MS Server" and "MV Full City" accident. See Table 7.2 for remark.

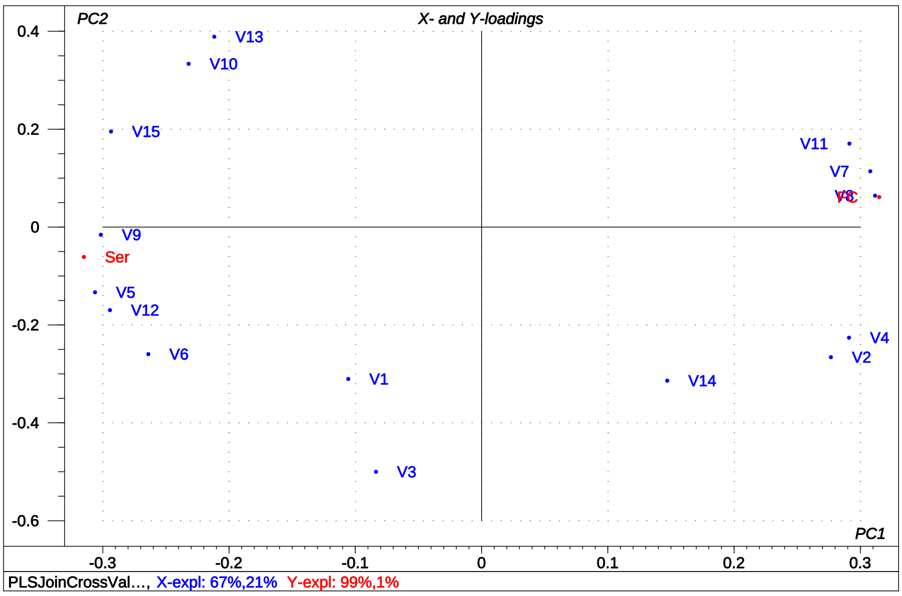

Figure 7.3: Loading plot PLS conducted to combined data from "MS Server" and "MV sFull City" accident. See Table 7.3 for remark.

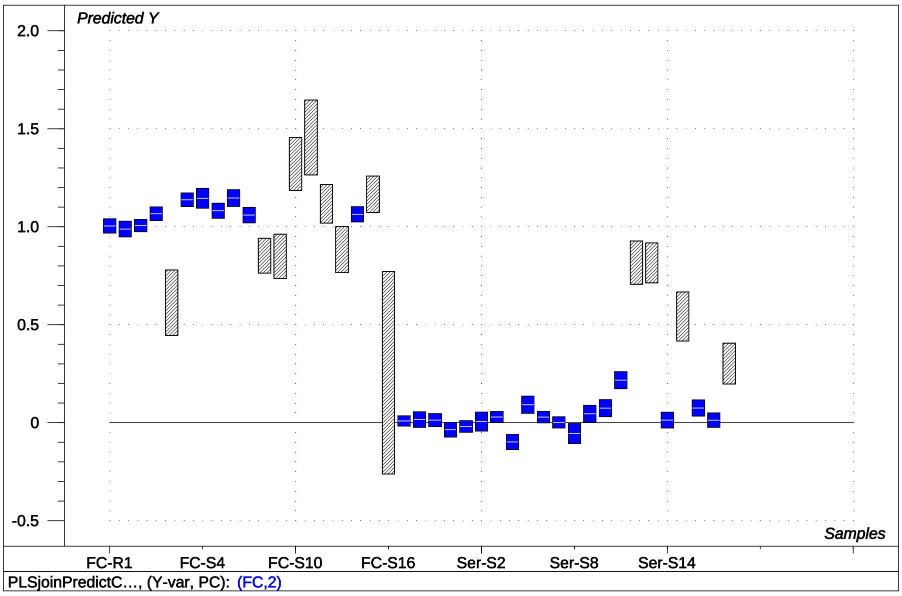

Figure 7.4: Predicted vs measured plot PLS conducted to combined data from "MS Server" and "MV Full City" accident. See Table 7.2 for remark.

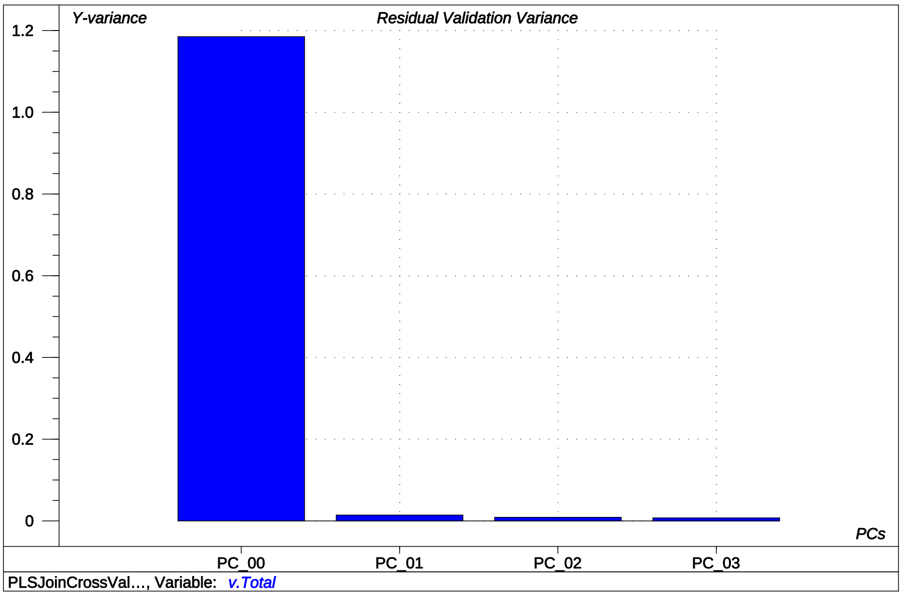

Figure 7.5: Residual variance plot PLS conducted to combined data from "MS Server" and "MV Full City" accident. See Table 7.2 for remark.

Table 7.2: Sample for PLS-DA applied to a combination of "MV Full City" and "MS Server" data set

Remark	Sample Name	Remark	Sample Name
FC-R1	Krogshavn	Ser-R1	Fedje
FC-R2	Oddane	Ser-R2	rom 3
FC-R3	Sastein	Ser-R3	rom 4
FC-S1	Mandal	Ser-R4	KV Eigun
FC-S2	Lekter	Ser-S1	rom 2
FC-S3	Nevlunghavn	Ser-S2	Teflon Herdla vest
FC-S4	Langesund bad	Ser-S3	Kelp Herdla Vest
FC-S5	Grimstad	Ser-S4	Gudbrandsøy
FC-S6	Risor	Ser-S5	oil Selje
FC-S7	Arendal	Ser-S6	oil Kvamsøy
FC-S8	Lasterom2	Ser-S7	oil Stongholmsvikjo
FC-S9	Lasterom 4	Ser-S8	oil Ivasanden
FC-S10	Maskinrom	Ser-S9	Bird Gannet
FC-S11	IFO180Vysotsk	Ser-S10	Bird Guillemot
FC-S12	LS180 Skagen	Ser-S11	Bird Osnessanden
FC-S13	HS180 Skagen	Ser-S12	Birds Lurøy
FC-S14	Lillesand	Ser-S13	birds Træna
FC-S15	Rockness	Ser-S14	oil Herøy
FC-S16	Askoy	Ser-S15	Oil Gryllefjord
		Ser-S16	Oil Vetvika
		Ser-S17	Oil Fyrsundet
		Ser-S18	teflon pad Fedje

Fig.7.2 is the score plot of the model. This figure shows clear separation between "MV Full City" class and "MS Server" class. The loading plot shown in Fig.7.3 shows that oil from "MV Full City" is determined by variable 29ab, B(a)F/4-Mpy, TA26, and 1Mpy/4-Mpy, whilst oil from "MS Server" is determined by variable C3-dbt/C3-phe, 4-MD/1-MD, C2-dbt/C2-phe and 27Ts. Predicted v.s. measured plot presented in Fig7.4 also shows clear separation between "MV Full City" and "MS Server" class. Residual variance in Fig.7.5 shows the optimal PC number, which is equal to 2.

The prediction step was then applied to all samples from "MV Full City" and "MS Server" accident. The result is shown from Fig.7.6-7.7.

Prediction with deviation is shown in Fig.7.6 for Y variable "MS Server". This figure is useful to define the member of "MS Server" class. Sample with $Y_{pred} > 0.5$ and low deviation is predicted as member of the class. These samples are references samples of "MS Server", which were taken from room 2,

Table 7.3: Variable name for PLS-DA applied to combination of "MV Full City"

Remark	Variable name
V1	1 Mpy/4-Mpy
V2	4-MD/1-MD
V3	2-MP/1-MP
V4	2Mpy/4-Mpy
V5	27bbSTER
V6	29ab
V7	29bbSTER
V8	29bb
V9	C3-dbt/C3-phe
V10	B(a)F/4-Mpy
V12	28bbSTER
V13	TA27
V14	27Ts
V15	TA26
V16	B(b+c)F/4-Mpy

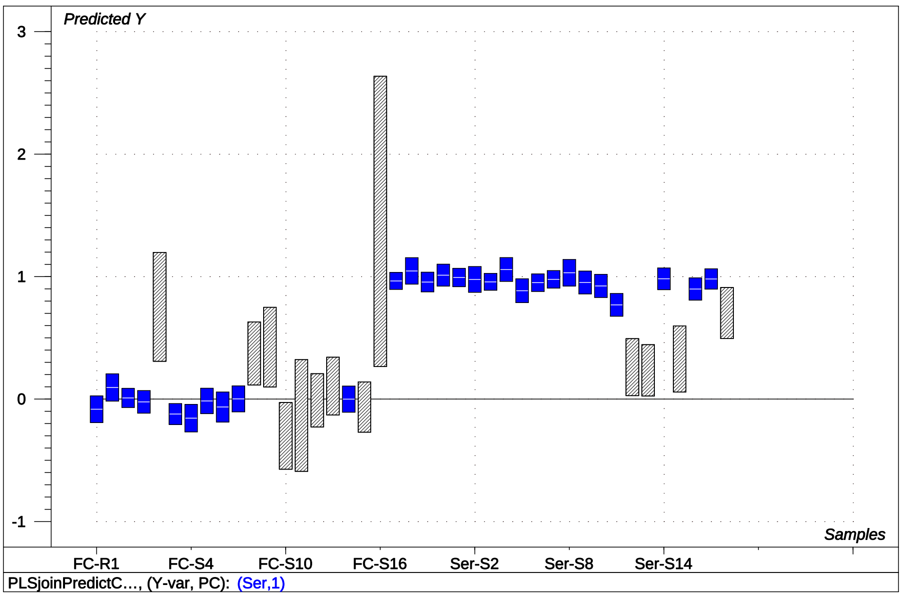

Figure 7.6: PLS prediction with deviation performed on combined data from "MS Server" and "MV Full City" accident for "MS Server" as Y variable. See Table 7.2 for remark.

kelp sample from Herdla vest, oil sample from Gudbrandsøy, oil sample from Selje, oil sample from Kvamsøy, oil sample from Stongholmsvikjo, oil sample from Ivasanden, bird feather sample from Gannet, bird feather sample from Guillemot, bird feather sample from Osnessanden, oil sample from Herøy, oil sample from Vetvika, and oil sample from fyrsundet. Sample with $Y_{pred} < 0.5$ and low deviation is predicted as non member of the class. This prediction shows that all samples taken from "MV Full City" accident are not member of "MS Server" class or not match to "MS Server". Samples with high deviation could not be safely classified in any class. This figure shows sample with high deviation, i.e. sample from Lekter, Langesund bad, Lasterom2, Lasterom4, machine room, IFO180, LS 180, HS 180, Rockness and Askøy from "MV Full City" accident and teflon pad sample taken from Fedje, birds feathers sample taken from Lurøy and Traæna, and oil sample from Gryllefjord from "MS Server"accident. The deviation is an uncertainty limit. If the X-data for the prediction sample is very similar to the training X-data, the deviation interval will be smaller and the prediction becomes more reliable. The larger deviation, the new sample is more dissimilar with the training sample [Esbensen et al., 1994]. Therefore, these samples are then concluded as not match to "MS Server" oil.

Prediction with deviation for Y variable "Full City" is shown in the Fig.7.7. This figure is useful to define the member of "MV Full City" class. In this figure, the predicted members are the reference samples from "MV Full City", sample taken from Mandal, Nevlunghavn, Langesund bad, Grimstad, Risør, Arendal, and Lillesand.

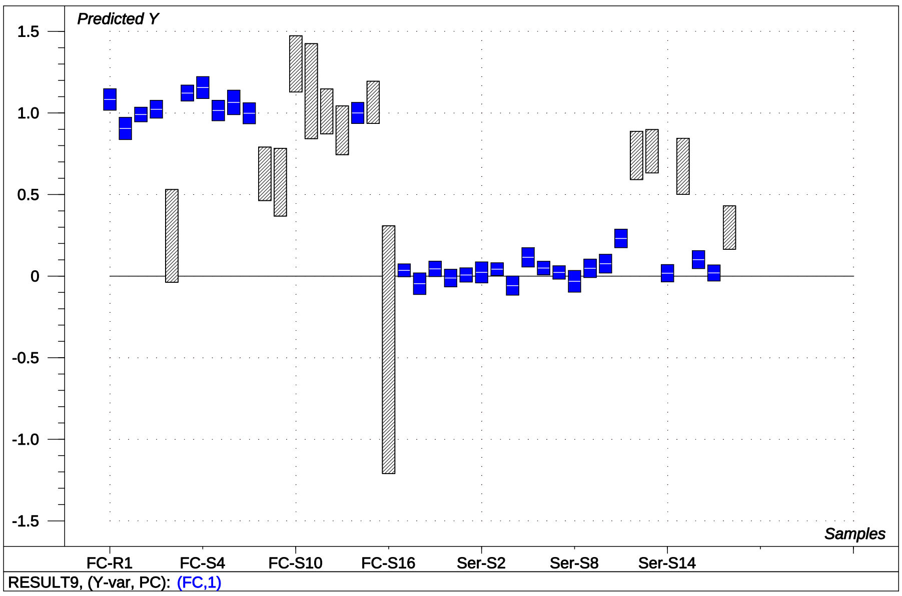

Figure 7.7: PLS prediction with deviation performed on combined data from "MS Server" and "Full City" accident for "Full City" as Y Variable. See Tab.7.2 for remark.

All samples taken from "MS Server" accident have $Y_{pred} < 0.5$ and low deviation so that predicted as non member of the class. Whilst, sample taken from

"MV Full City", sample taken from "Rockness" accident, IFO 180 Vysotsk, LS 180 Skagen, and HS 180 Skagen have large deviation and therefore concluded as not match to "MV Full City" oil.

8 COMPARISON AND DISCUSSION

8.1 GENERAL COMPARISON

CEN-method for oil spill forensic is a standardized method for oil spill fingerprinting in Europe. The application of this method is intended to assure standard and uniform procedure on the oil spill examination, such that an oil spill can be classified as identical or not identical to the suspect/source samples. Basically, this method can be performed without any special software, such that can be easily applied by any analyst. However, this method requires diagnostic ratio (DR) comparison one by one, such that it takes more time as compared to the multivariate one. This can increase the cost of man hour. More comments regarding this method is given later in Sect.8.2.

Several multivariate analyses in this thesis were performed using a software called *The Unscrambler*. This software has been used by SINTEF as a tool for oil spill related matter including oil spill investigation and has given satisfied results. Special expense for this software or perhaps other statistical softwares is needed and therefore it could be problem for others in elsewhere in the world to acquire such softwares. A special skill for operating the software is also needed. Fortunately, *The Unscrambler* has complete user manual and technical guidelines so that a new user can learn this software easily. Another problem related to application of multivariate analyses using special software is availability. Not every research institute or laboratory in the world has special statistical software that suitable for oil spill investigation. Therefore, when an oil spill occurred at the place where this software is not available, this technique can not be easily applied. In this case, open source statistical softwares can be used as alternatives.

Other requirement for oil spill investigation results can be accepted is its simplicity to explain in front of the court and public. In this case, CEN standardized method tends to be easier rather than any multivariate method. CEN-method requires to compare spill sample and the reference sample in one-to-one comparison, a variable by a variable, so that easy to be understood. For most of the people, multivariate analysis is a sort of throwing in many numbers to a black box in order to obtain another numbers, which then interpreted subjectively by the analyst. For the case of oil spill fingerprinting, many numbers (in this case is DR) from various samples were thrown together into multivariate software in order to obtain a pattern, which is then used for deciding whether an oil spill sample is match or not to the reference sample. Even though the process inside a multivariate software can be explained mathematically, but it is still too complex for common people. Therefore, there is a tendency that multivariate analysis is more difficult to be defended in front of the court as compared to the CEN-method.

Table 8.2: Result comparation of CEN standardized method, PCA combined with cluster analysis and PLS-DA for "Full City" Case

Sample ID	Location	CEN (Author)	CEN SINTEF	PCA_CA Scale	PCA-CA Unscale	PLS - DA
2009-0472	Oddane	Ref	Ref	Ref	Ref	Ref
2009-0473	Oddane	NM all	NM all	*	*	*
2009-0474	Oddane	*	M all	*	*	*
2009-0482	Krogshavn	*	M all	*	*	*
2009-0483	Krogshavn	*	M all	*	*	*
2009-0484	Krogshavn	*	M all	*	*	*
2009-0485	Krogshavn	NM Od & Sås	NM Od&Sås, M Krogs	Ref	Ref	Ref
2009-0486	Landoy/Mandal	PM to Od& Sås,NM to Krog	NM Od&Kros, M Sås	M Sås	M Sås	M
2009-0487	Hanestangen Kris- tiansand	NM all	NM All	*	*	*
2009-0489	Barge	NM all	NM all	*	*	*
2009-0490	Såstein	*	M All	*	*	*
2009-0491	Nevlunghavn	PM all	M to Sås	M Sås	M Sås	M
2009-0492	Krogshavn	*	M all	*	*	*
2009-0493	Langesund bad	NM all	M Krogs,	M to Krogs	M Krogs	M
2009-0494	Nevlunghavn	NM all	NM All	*	*	*
2009-0495	Mølen	*	M all	*	*	*

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Sample ID	Location	CEN (Author)	CEN (SINTEF)	PCA-CA Scale	PCA-CA Unscale	PLS - DA
2009-0499	Hassletangen Grimstad	PM Sås& Od,NM Krog	M Od	M Od&Sås	M Od&Sås	M
2009-0500	Fie/ Risør	PM all	M Od	M to Od&Sås	M Od&Sås	M
2009-0501	Arendal	M to Od, PM Sås&Krogs	M Od	M Od&Sås	M Od&Sås	M
2009-0518	Barge1	*	M All	*	*	*
2009-0521	Barge 1	*	M All	*	*	*
2009-0522	Barge 2	*	M All	*	*	*
2009-0525	Barge 2	*	M All	*	*	*
2009-0564	Såstein	Ref	Ref	Ref	Ref	Ref
2009-0579	Såstein	PM Od, M Sås, NM Krogs	PM Od, M sås, NM Krog	Ref	Ref	Ref
2009-582	Såstein	Ref	Ref	Ref	Ref	Ref
2009-0602	Cargo 2	PM Od, NM Sås, PM Krogs	NM all	NM	NM	NM
2009-0603	Cargo 3	*	M all	*	*	*
2009-0604	Cargo 4	PM Od, NM Sås & Krog	PM Od, NM Sås&Krog	NM	NM	NM
2009-0605	Cargo 5	*	M all	*	*	*
2009-0606	Machine room	NM all	NM All	NM	NM	NM
2009-0609	IFO180Vysotsk	NM all	NM All	NM	NM	NM
2009-0614	LS180 Skagen road	NM all	NM All	NM	NM	NM

Continued on Next Page…

Sample ID	Location	CEN (Author)	CEN (SINTEF)	PCA-CA Scale	PCA-CA Unscale	PLS - DA
2009-0616	HS180 Skagen road	NM all	NM All	NM	NM	NM
2009-0622	Lyngholm Lillesand	PM Od&Sås, NM Krogs	PM Od&Sås,NM Krog	M to Od&Sås	M to Od&Sås	NM
2009-0624	Napa, Vestfold	NM all	NM all	*	*	*
2009-0630	Barge 3	*	M all	*	*	*
2009-0634	Barge3	*	M all	*	*	*
2009-0736	Krogshavn	*	M all	*	*	*
2009-0737	Krogshavn	*	M all	*	*	*

M = Match

NM = Non Match

all = all reference samples

PM = Probable Match

Krogs = Reference sample from Krogshavn

Od = Reference sample from Oddane

Sås= Reference sample from Såstein

Table 8.3: Result comparation of CEN standardized method, PCA combined with cluster analysis andPLS-DA for "Server" case

Sample ID	Location	CEN(Author)	CEN SINTEF	PCA_CA Scale	PCA-CA Unscale	PLS - DA
2007-0010	KV Ålesund	*	M	*	*	*
2007-0011	KV Ålesund	*	M	*	*	*
2007-0012	KV Eigun	*	M	*	*	*
2007-0014	Pad Sample Fedje.	NM	NM	NM	NM	NM
2007-0015	Innarøyene.	*	M	*	*	*
2007-0016	area around the scrapped rock.	*	M	*	*	*
2007-0017	TV-bukta Fedje. Sample from Sturla Dyregrov.	R	*R*	R	R	R
2007-0018	Teflon pad, Herdla Vest	NM	NM	NM	M	M
2007-0019	Rullestein strand, Herdla vest.	PM	M	M	M	M
2007-0020	Sauøy (farm oygarden)	*	M	*	*	*
2007-0021	Lense, Gudbrandsoy	*	M	*	*	*
2007-0022	"Server": Sample from Tank 2	NM	NM	NM	NM	M
2007-0023	"Server": Sample from Tank 3	R	*R*	R	R	R
2007-0024	"Server": Sample from Tank 4	R	*R*	R	R	R

Continued on Next Page...

Sample ID	Location	CEN (Author)	CEN (SINTEF)	PCA-CA Scale	PCA-CA Unscale	PLS - DA
2007-0025	Selje kommune	NM	NM	M	M	M
2007-0026	Vagsoy kommune	*	M	*	*	*
2007-0027	Vagsoy kommune	*	M	*	*	*
2007-0028	Flora kommune	*	M	*	*	*
2007-0029	Flora kommune	*	M	*	*	*
2007-0030	Flora kommune	*	M	*	*	*
2007-0033	KV Eigun	R	*R*	R	R	R
2007-0042	Osnessanden, Ulstein Kommune	*	M	*	*	*
2007-0055	Fedje kommune	*	M	*	*	*
2007-0056	Gullbransoyna, Post 4	*	M	*	*	*
2007-0057	Radoy, Syltavegen	*	M	*	*	*
2007-0058	Radoy /Marøy/Leitevegen	*	M	*	*	*
2007-0059	MS Server, Gulen	*	M	*	*	*
2007-0060	MS ServerGulen	*	M	*	*	*
2007-0061	MS Server, Gulen	*	M	*	*	*
2007-0062	birds (gulls)Onoy, Luroy	NM	NM	NM	NM	NM
2007-0063	Kvamsoy, Sande Kommune,	PM	M	M	M	M

Continued on Next Page…

Sample ID	Location	CEN (Author)	CEN (SINTEF)	PCA-CA Scale	PCA-CA Unscale	PLS - DA
2007-0064	Stongholmsvikjo, Bomle kommune	PM	M	M	M	M
2007-0065	Ivasanden, Ulstein	PM	M	M	M	M
2007-0066	Bird feathers from gannets Ivasanden, Ulstein	PM	M	M	M	M
2007-0067	Bird feathers from guillemot / razorbills, Ivasanden, Ulstein	PM	M	M	M	M
2007-0068	Bird feathers from dead eiders Osnessanden, Ulstein	NM	M	M	M	M
2007-0069	Hamsundpollen, Hamaroy kommune.	*	No oil	*	*	*
2007-0070	Bird feathers Træna	NM	NM	NM	NM	NM
2007-0084	Okstadvika, Heroy	NM	M	M	M	M
2007-0105	Eide, 9380 Gryllefjord	NM	NM	NM	NM	NM
2007-0118	Austrheim	*	PM	*	*	*
2007-0119	Austrheim	*	PM	*	*	*
2007-0282	Vetvika, Bremanger kommune, Nordfjord	PM	M	NM	M	M
2007-0394	Fyrsundet position 2, Fedje	PM	M	NM	M	M

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Sample ID	Location	CEN (Author)	CEN (SINTEF)	PCA-CA Scale	PCA-CA Unscale	PLS - DA
2007-0395	Fyrsundet position 2, Fedje	PM	M	NM	M	M

M = Match

NM = Non Match

PM = Probable Match

Comparison of the results of oil spill fingerprinting for oil spill case studies "MV Full City" and "MS Server" by means of standardized CEN-method and several multivariate methods are tabulated in Table 8.2 and 8.3. Detail explanation of the result of each method is explained in the Sect.8.2-8.5.

It is noted in the tables that some samples are marked by "*" indicating no available diagnostic ratio data and therefore no comparison was made. Comparison between CEN-method and multivariate methods only valid for samples which have diagnostic ratio data. Some discrepancies between the CEN-method applied by the author and the one applied by SINTEF are observed and will be explained later on in Sect.8.2.

8.2 CEN METHOD FOR OIL SPILL FORENSIC

This method, as described in Sect.2.3, involves three levels of examination, i.e. GC-FID chromatogram visual inspection (level 1), GC-MS chromatogram visual inspection (level 2), and diagnostic ratio evaluation (level 3). This section is intended to describe the problems or drawbacks when performing oil spill fingerprinting by means of CEN-method.

Several problems were experienced by the author when applying the CEN-method upon both oil spill cases ("MV Full City" and "MS Server"). The first problem was when deciding which samples should be continued to the second level after the evaluation of GC-FID chromatogram (level 1). Actually CEN-method stated that sample which has no different on GC-FID chromatogram pattern, or the pattern differences were caused by weathering processes, should continue to the next level. However, the application of the method by SINTEF seems to be deviate due to consideration of other factors, such as examination cost, history of the sample, etc. The consideration can be observed from some samples which has no different on GC-FID pattern with the reference samples, but they were not considered to the next examination level. This was somehow deviate from the CEN-method guideline.

For example, in "MV Full City" case, samples numbered SINTEF ID 2009-0474, 2009-0482, 2009-0483, 2009-0484, 2009-0518, 2009-0521, 2009-0522, 2009-0525, 2009-0603, 2009-0605, 2009-0630, 2009-0634, 2009-0736, and 2009-0737 were concluded as match to the reference samples, without conducting further analyses in level 2 and 3 (as supposed to be, according to the CEN-method). These samples were taken in the ship and at the area which are highly affected by oil spill (Oddane and Krogshavn). This decision somehow understandable that no need for further examination when in fact those spill samples were indeed taken from the wreck and surrounding it. This sort of consideration somehow reflects the importance of sample history in the analysis.

A contradicting consideration is also observed in "MS Server" case. Samples numbered SINTEF ID 2007-0070, 2007-0084, 2007-0105, 2007-0062, 2007-0014 were in fact continued to the next level of examination even though the GC-FID inspection (level 1) showed that they have different pattern and the differences were not caused by weathering processes. While according to the CEN-method, those samples should be directly marked as non match. In this case, there was no obvious reason apparent to the author.

The first problem as described in the previous paragraphs leads to a conclusion that there are different basic ways of thinking between the CEN-method and SINTEF approach, even though both apply 3 levels of examination. This statement is especially true when learning the "MS Server" case. CEN-method starts the examination by assuming that the oil spill is basically non match. Therefore, when level 1 examination concluded that the sample is match, the sample should go through the next levels of examination until at the end of the examination in level 3. A sample considered as match if all of those 3 levels of examination conclude it to be match. This way of thinking somehow seems to be in favor of the shipowners and/or the culprit. However, the benefit of this approach is the conclusion will be very strong and undeniable, which is especially needed in front of the court.

While SINTEF approach seems to be started by prejudgment that the collected oil spill sample should be from the suspected/reference samples. Therefore, once level 1 concluded that the spilled sample is match, then it is enough to mark it as match and no further examination is needed. But, if level 1 examination concluded otherwise, then more analyses in the next levels are required until at the end of the examination in level 3. A sample considered as non match if all of those 3 levels of examination concluded it to be non match. This way of thinking somehow seems to be in favor of the environment and regulatory bodies. However, the drawback of this approach is the conclusion somehow has lower confidence level and it could be a quite setback in front of the court.

The deviated approach by SINTEF with respect to the CEN-method on handling the "MS Server" case leads a problem when the author conducting this work. This is because the work by author depends on the data (either GC-FID chromatograms, GC-MS chromatograms, and diagnostic ratio) provided by SINTEF report. When SINTEF [Almås et al., 2007] decided to title match to the sample in level 1 and then discard it from level 2 and 3 examinations, it means that there is no available GC-MS chromatograms and diagnostic ratio data for the corresponding sample. Therefore, no data means no analysis can be done by the author for particular samples. Samples undergo this condition were consecutively marked with "$*$" in Table 8.2 and 8.3. This case of course hindered the final conclusion of the investigation in this thesis.

The second problem was diagnostic ratio calculation. Miss-application of the equation to be used for the calculation of diagnostic ratios sometimes happened, as describe in Sect.4.3.2. This problem can be solved by creating a program or excel spreadsheet that can automatically generate diagnostic ratio based on the responses of GC-MS chromatogram. This has been performed by the author using *MATLAB*. Other mathematical softwares, such as *Python* or *Octave*, can be used as an alternative.

Knowledge about the type of oil being investigated is also plays an important role in selecting diagnostic ratio for evaluation. For example in the "MV Full City" case, SINTEF did not included several diagnostic ratios such as DR

-Retene/C4-Phe. It was noted that "MV Full City" contains IFOs oil type which were produced in high temperature process. Retene is aromatic compound with slightly longer side chains and therefore will not occur in IFOs oil type [Al-Khudhairy, 2006]. This information was not known in advance by the author. Therefore, the author still used this DR for matching process. This was of course lead to different and wrong conclusion in oil spill forensic. More over, this case nevertheless supports Christensen and Tomasi [2007] opinion that no matter how powerful and refined univariate method for oil spill fingerprinting, even the standardized one (CEN-method), relies on expertise and skill of the analyst.

Interestingly, comparison of the result between CEN-method performed by the author and the one performed by SINTEF also shows that CEN-method relies on expertise and skill of the analyst. CEN-method for oil spill forensic performed by SINTEF gave more reliable result as compared to the author results. This kind of conclusion was confirmed later by other methods, such as PCA combined with cluster analysis and PLS-DA. SINTEF result gave more similar result to the result of these methods.

8.3 principal component analysis for oil spill forensic

PCA for oil spill fingerprinting has been applied since in the middle of 1990s [Christensen and Tomasi, 2007]. Al-Khudhairy [2006] also suggest to perform PCA to support the result of the CEN-method of oil spill fingerprinting. PCA is a multivariate statistical method that creates new independent variables, which are linear combination of original variables. In this method, relationships between similar objects can be found. This is useful for matching process in oil spill identification.

In this thesis, this matching process was performed by score plot visual inspection. This method was very easy to be applied, but sometime it was difficult to be performed because the objects formed clusters with different shapes and densities [Bratchell, 1992]. This difficulty also occurred when this method was applied to the "Full City" and "Server" oil spill case. This problem can be solved by other classification multivariate method, such as cluster analysis (see Chapter 6). Moreover the objectivity of matching process of spill and source oil samples can be improved by numerical comparison or statistical test [Christensen and Tomasi, 2007].

Using PCA loading plot, contribution of variables in the samples can be explained. This is useful for the analyst. Especially when the knowledge of the sample to be used for the analysis is limited. For example, loading plot shown in Fig.5.5 and Fig.5.8 shows high contribution of 2-MP/1-MP. This diagnostic ratio was generated from M-phenanthrenes. The cluster of isomeric M-phenanthrenes is typical of the high-temperature production of aromatics, such as IFO oil type [Al-Khudhairy, 2006]. This information is useful for oil spill investigation and can be easily obtained by inspection of PCA loading plot.

Data pre-processing plays important role for oil spill forensic using PCA. Different pre-treatment of the data will lead to different conclusion and moreover can give wrong conclusion. In this work, both scaling and un-scaling the variables were performed to the data as pre-treatment. In "MV Full City" case, there are no discrepancy in concluding match or non match of the sample to the references. But in "MS Server"case, application of scaling and un-scaling the variables lead to different final conclusion. In "MS Server" case the application of un-scaled variables give more similar result with CEN-method conclusion performed by SINTEF as compared to the scaled ones. This finding also lead to suspicion that the discrepancy also due to lack of the available data (GC-MS chromatogram and DR data), see Sect.8.2. Therefore, it is important to specify that comparison of the PCA result with CEN-method for oil spill only valid for samples that were undergo GC-MS examination.

In this master thesis, PCA was performed using statistical software called *The Unscrambler*. This software is user friendly but of course take more cost as compared to the analysis using CEN-method, which can easily be performed using excel spreadsheet or any numerical analysis software such as *MATLAB* or *Python*. Developing a specialized software for oil spill fingerprinting, including CEN univariate and multivariate statistical analysis, can be proposed for further work to reduce cost and generate more reliable and robust result.

8.4 HIERARCHICAL CLUSTER ANALYSIS

Hierarchical cluster analysis is an unsupervised classification method. This method is able to find natural classes or clusters in the data by measuring similarity or dissimilarity. This feature is useful for matching process in oil spill forensic.

Selection of linkage, i.e. cluster distance measure to be used for hierarchical cluster analysis, is important. Hierarchical cluster analysis using Euclidean distance complete linkage shows more reliable result as compared to the two other linkages. This is because in this method, the distances between clusters are determined by the greatest distance between any two objects in the different clusters (i.e. by the "furthest neighbors"). Therefore, it performs quite well in cases when the objects actually form naturally distinct "clumps" [Statsoft, 2011], such as in oil spill fingerprinting case.

Cluster analysis gives straightforward and intuitive interpretation on the sample classification. However the contribution of variables in each class or cluster is not known by this method. Since cluster analyses for oil spill forensic applied in this thesis are applied only for supporting method to classify samples based on PCA scores, further application for the more raw data, i.e diagnostics ratio, is strongly suggested.

8.5 PARTIAL LEAST SQUARE-DISCRIMINANT ANALYSIS

Application of PLS-DA in oil spill investigation is relatively rare. This thesis compared this method with other more common methods, i.e CEN standardized method and PCA. Again, this comparison is only valid for samples that were analyzed using GC-MS or samples with known diagnostic ratio values.

PLS-DA results depend on the selected validation. Even though cross validation can be used for validation of classification model using small number of sample, this validation only gives a reliable result when proper procedure is performed. In the proper cross validation procedure, the total data should be divided into a training set, a validation set, and a test set [Westerhuis et al., 2008].

Application of PLS-DA by combining datasets from "MV Full City" and "MS Server" has enabled the division of the data into training set, validation set and test set. For "MV Full City" case, the application of PLS-DA resulted the same conclusion as produced by the CEN-method performed by SINTEF and PCA combined with cluster analysis. Whilst, limitation of PLS-DA in this case was unable to identified a specific spill sample to be match with a specific reference sample. This was because the number of reference sample from "MV Full City" was too small, such that not possible to divide the reference samples into three classes and performing PLS-DA only on "MV Full City" case. Increasing the number of reference sample could be a solution for this problem.

For "MS Server" case, there are some discrepancies between the result of this method with both by CEN-method and also using PCA combined with cluster analysis. PLS-DA predicts the oil samples taken from room 2, teflon pad sample from Herdla Vest, and oil sample from Vetvika are member of "MS Server". These samples were actually identified as non match by CEN-method. PLS-DA prediction also shows discrepancies with PCA result, especially when PCA is performed with autoscaling the variables. These discrepancies could be because of different variables being used for the analysis. As described in Chapter 7, some variables were removed in order to combine these two data sets. The discrepancies also could be because too few number of samples to be used for building the model, which were only 7 samples. Again, this problem can be solved by increasing number of samples to be used for building the model. This is of course will increase the cost, especially when number of samples needed for analysis is not known. In this case, the author suggests Monte Carlo simulation for determining the appropriate number of samples especially source or reference samples [Westerhuis et al., 2008].

9 CONCLUSION AND FUTURE WORKS

9.1 CONCLUSION

A hypothesis as starting point of this thesis was that the CEN-method for oil spill fingerprinting (even though can be done easily by a calculator or excel spread sheet) depends on the expertise of the analyst. This made the method less objective. The hypothesis above turned out to be true when the author (who has limited skill and experience) conducted the oil spill fingerprinting based on CEN-method for "MS Server" and "MV Full City" oil spill cases, see Sect.3 and 4. When the result was compared with the SINTEF result, some discrepancies were revealed. It was a sort of indication that the skill level and experience of the analyst does matter and important for the consistent conclusion when applying the CEN-method, see Sect.8. Moreover, it was found that the univariate CEN-method tends to take longer time as compared to the multivariate methods because matching process of spill sample and reference sample is done in one-by-one basis. This will increase the cost of man hours, and could be more expensive as compared to the procurement of any multivariate software.

In this thesis, multivariate analyses using PCA, cluster analysis and PLS-DA (see Sect.5,6, and 7) have been proven as faster and undoubtedly more objective as compared to the CEN-method. The gap of the skill level and experience of the analyst is no longer matter. This has been demonstrated by more similar result when compared with the SINTEF's. These benefits consequently give another benefit, such as reduce the cost for man hours. The limitations of these method are the cost needed for software expense and in some places of the world, the availability of the software could be a problem. Another limitation of the multivariate analysis application is its complexity. This complexity tends to be more difficult to be defended in front of the court as compared to the univariate one (CEN-method) due to lack of one to one comparison.

Throughout the case studies, this work shows that PCA is able to be used to classify whether a spill sample match or not to the reference sample by visual inspection of score plot. However, in several cases, the objects lay in a scatter way and therefore it is difficult to conclude whether a spill sample is match to the reference sample or not. The author found that by combining PCA with cluster analysis, the difficulty can be solved. However, the difference in data pretreatment (i.e. by performing auto-scaling or not) tends to give different conclusion. It means good knowledge about the effects of the data pretreatment is required. It seems that further research in this area is needed.

The last multivariate analysis investigated by the author was PLS-DA, which demonstrated even closer result to the CEN-method performed by SINTEF as compared to the PCA combined with cluster analysis. This method could be considered to be more objective and confidence to predict whether a spill sample match to the reference sample or not. Therefore, the author recommends to use this method for DR evaluation in oil spill investigation, rather than the method explained in Al-Khudhairy [2006], which uses repeatability limit for diagnostic ratio comparison, or PCA combined with cluster analysis. However, this method seems to be depend on the number of sample to be used for building the model. The consideration regarding the number of sample to be used for PLS-DA somehow relates to the cost. The more number of sample means the more cost for chemical analysis is needed. The optimum number of sample and other related features should be investigated in the future work.

9.2 FUTURE WORKS

Since there is discrepancy on calculation of diagnostic ratio (DR) between the author and SINTEF, the author suggests to increase the accuracy of DR calculation by developing software that can automatically generate DR from response/peak data of GC-MS. The author also suggests to improve the use of more "raw" format GC-FID or GC-MS data for oil spill investigation. The using of this data is expected to be able to improve the time efficiency, and also to be able to reduce error on DR calculation.

In this thesis, several multivariate analyses are performed using a software called *The Unscrambler*. For some parts of the world, the using of a licensed software could be difficult and the expense to acquire it could be a problem. This problem can be solved by performing multivariate analysis in an open source chemometric software, such as *SciCraft*. Otherwise, developing a specialized purpose software for oil spill investigation could be beneficial and can be subjected for further work.

Other multivariate analyses for classification such as Soft Independent Modeling of Class Analogy (SIMCA) is also suggested to be considered as further work. This approach has a goal to assign a new sample to the class with the largest similarity. This type of classification is based on separate PC models, usually separate PCA model. The method consist of two stages, i.e training stage and classification stage. Different distance measures are used to evaluate the class membership of new object. Therefore, classification of the new sample in to any class can be performed easily [Esbensen et al., 1994].

Among several multivariate analyses performed in this thesis, PLS-DA is one of the promising method for oil spill investigation. However, the optimum number of sample for analysis in order to obtain a valid model and consistent result is remain a problem. Further work should be done to figure out the optimum number of sample for PLS-DA for various oil spill cases.

It should be understood that this thesis has been build up upon the available data only, which is a real oil spill case. The problem of building up of a conclusion or theory based on a real case study is we cannot sure about the "truth" 100% we might found, because everything tends to be uncontrollable. The more appropriate approach in order to pursue an alternative or complementary method of the univariate CEN-method is by performing this investigation upon more controllable samples. Controllable sample means that the oil type and its components are known. Moreover, the type of weathering process and its severity with respect to the time of exposure to the weathering process is also known. An artificial weathering process can be imposed to the sample to imitate the real weathering process in more controllable way. If the whole work in this thesis is performed upon such controllable samples, the conclusion will be strong and undeniable.

Moreover, we could simulate several types of weathering processes to several oil types or even in a mixture of oil types and then investigate it using GC-FID and GC-MS. Finally, we could establish a very important database, which contain information of components in each oil type and the effect of weathering degree to the oil component. Using PLS-DA, we can build models from this databases and predict whether an illegal oil spill matching to one of oil type we have modeled or not.

Application of PLS-DA with other analytical method which is more practical could be considered as further work. This application will enable to develop an apparatus that can be used to investigate whether a spill match to any type of oil or not on site. This is of course will increase the time efficiency, because the spill sample is not necessary to be analyzed in the laboratory and also avoid the mixed up of oil samples. Therefore, it will increase the objectivity of oil spill investigation.

A

CEN LEVEL I - GC/FID VISUAL INSPECTION: "FULL CITY" CASE

For "Full City" case, based on GC/FID analysis result done by SINTEF [Faksness et al., 2010], which was available in form of figures in pdf file (no digital data available), the author digitized all GC/FID chromatogram of the samples by mean of graph digitizing software, *windig25*. Afterward, Level 1 screening by overlaying the chromatogram of the spill sample on top of the reference sample could be easily performed in Matlab. The results are presented in this appendix.

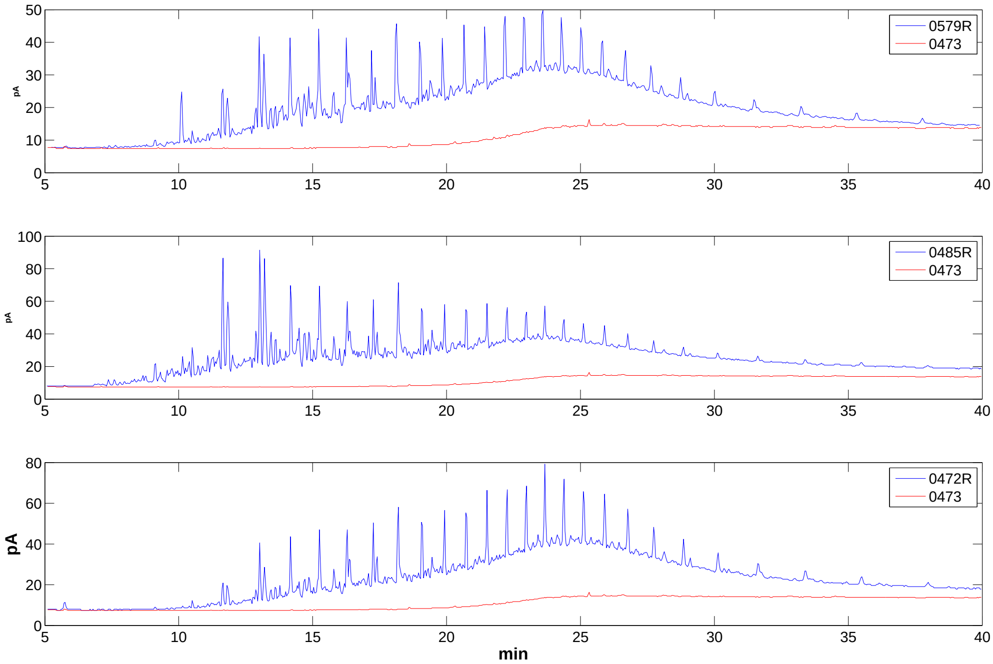

Figure A.1: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0473) and the reference samples.

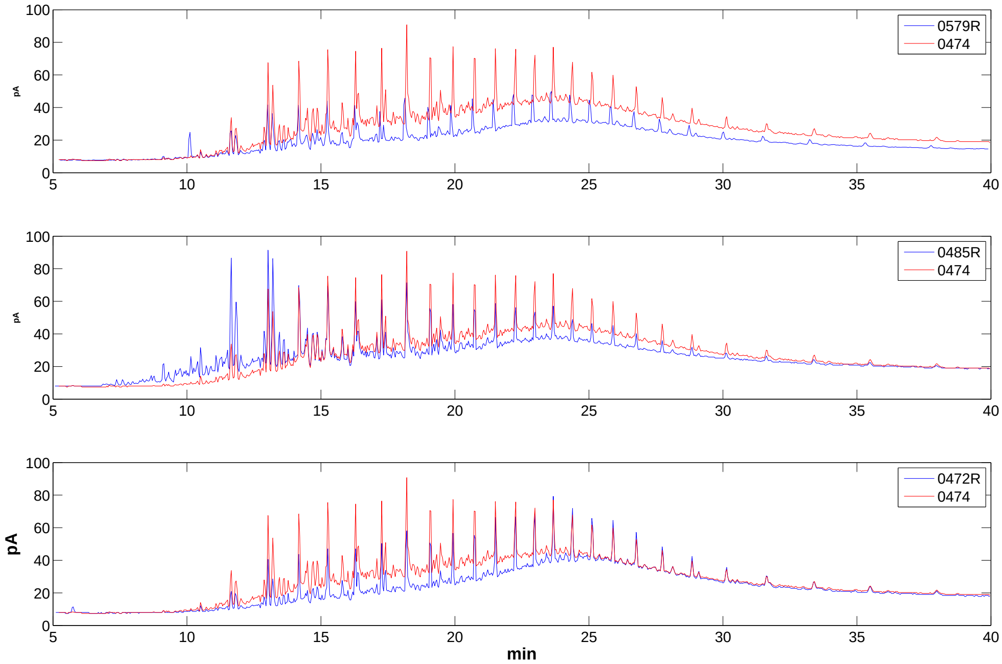

Figure A.2: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0474) and the reference samples.

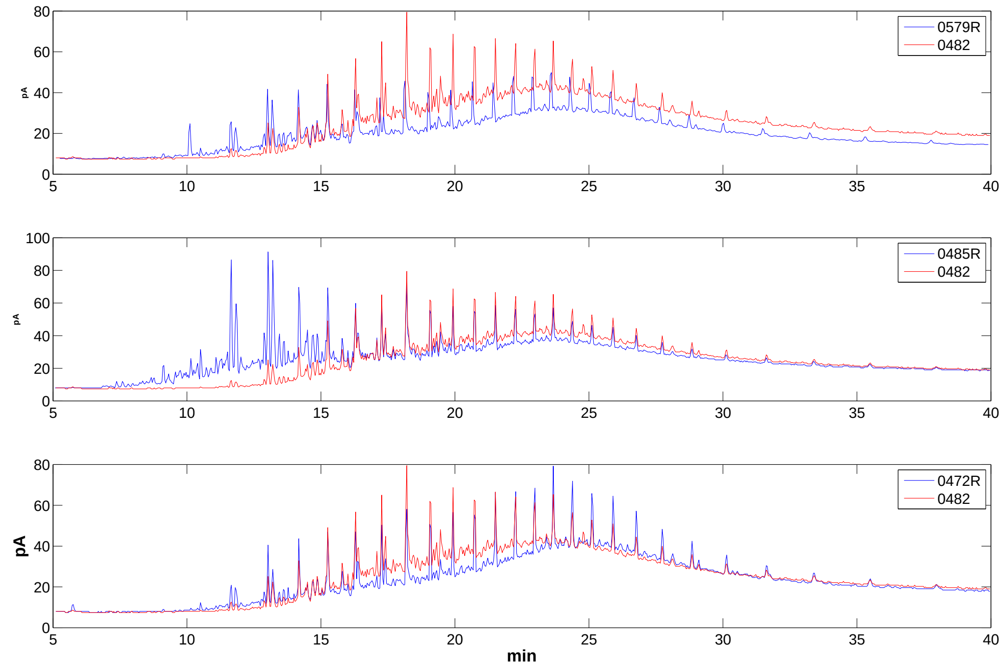

Figure A.3: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0482) and the reference samples.

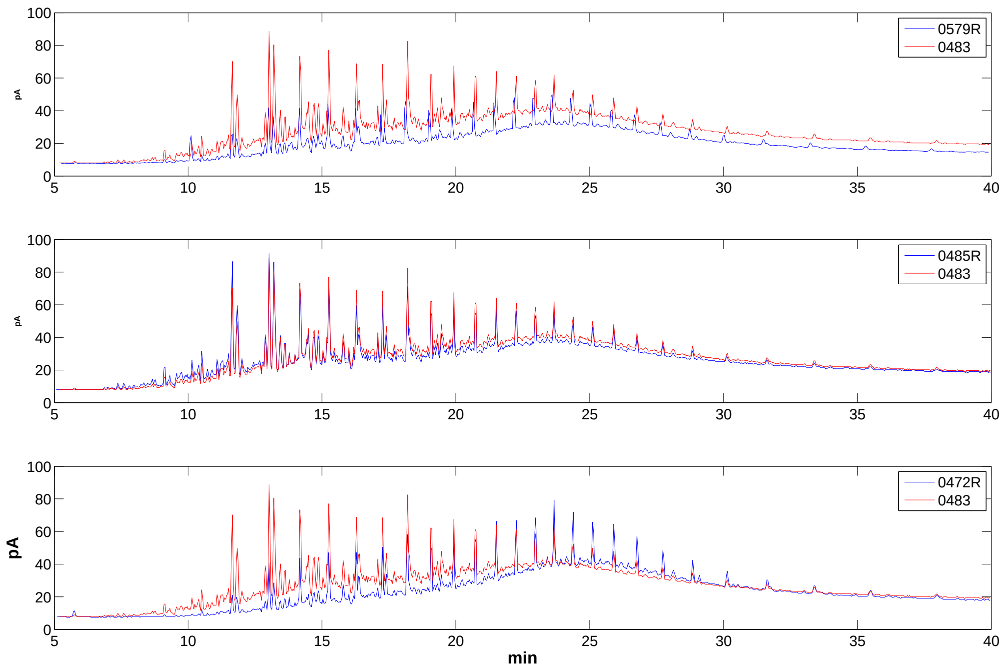

Figure A.4: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0483) and the reference samples.

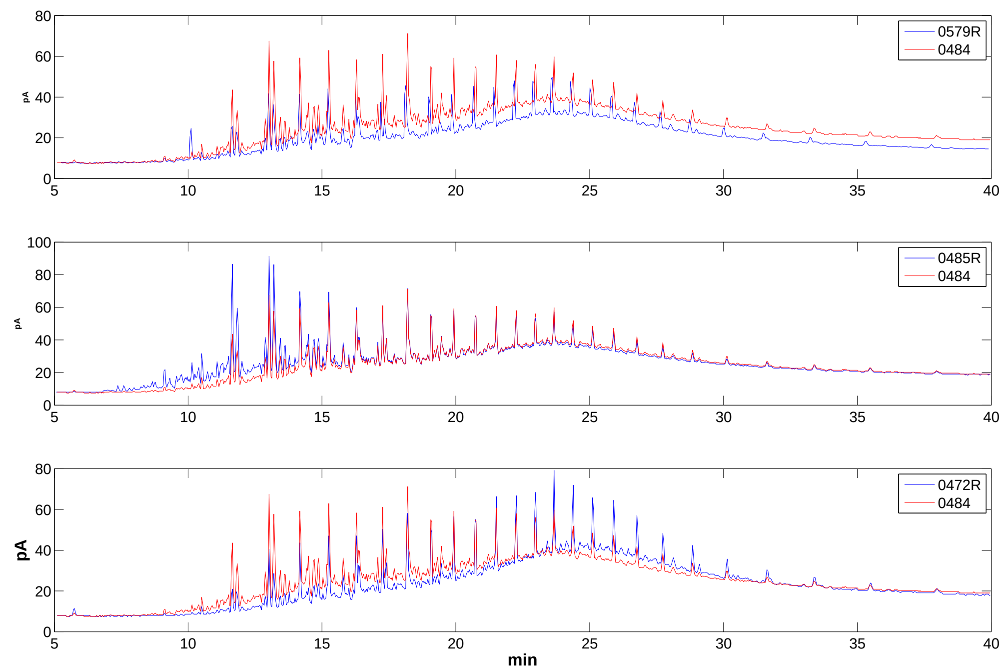

Figure A.5: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0484) and the reference samples.

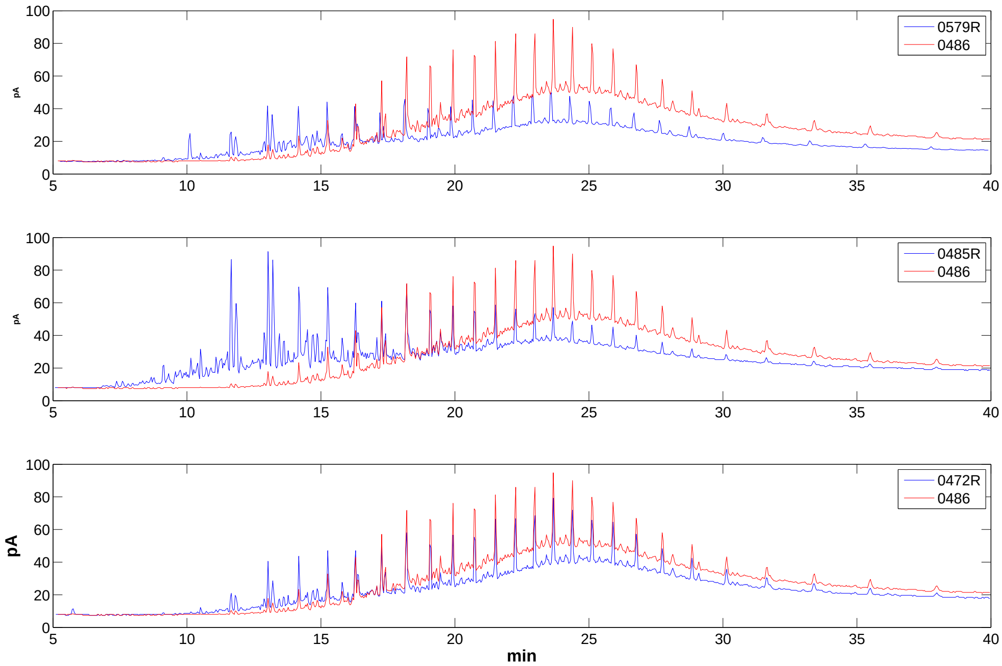

Figure A.6: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0486) and the reference samples.

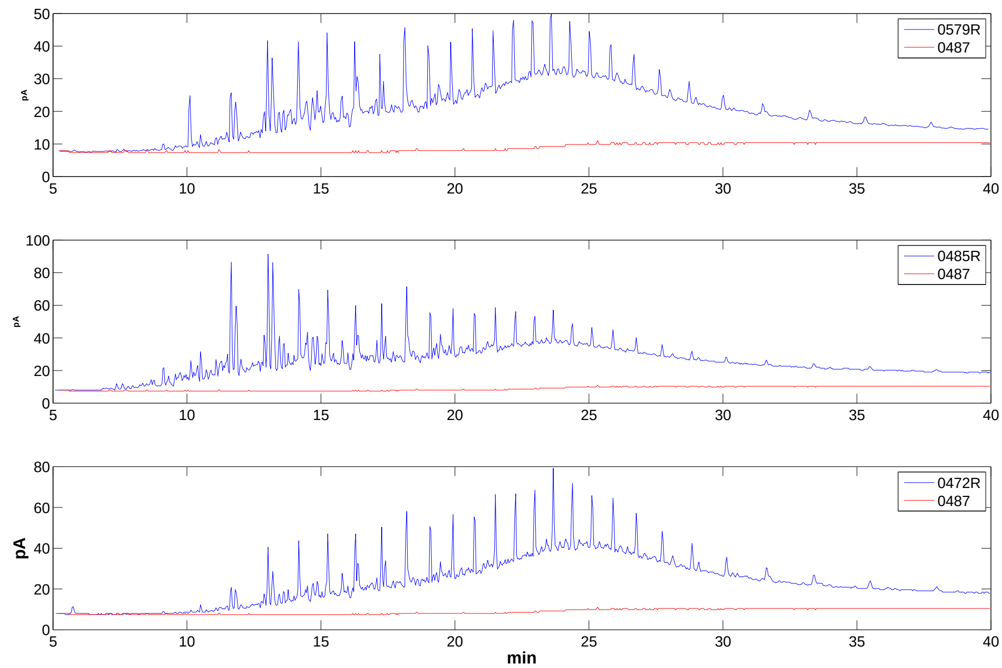

Figure A.7: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0487) and the reference samples.

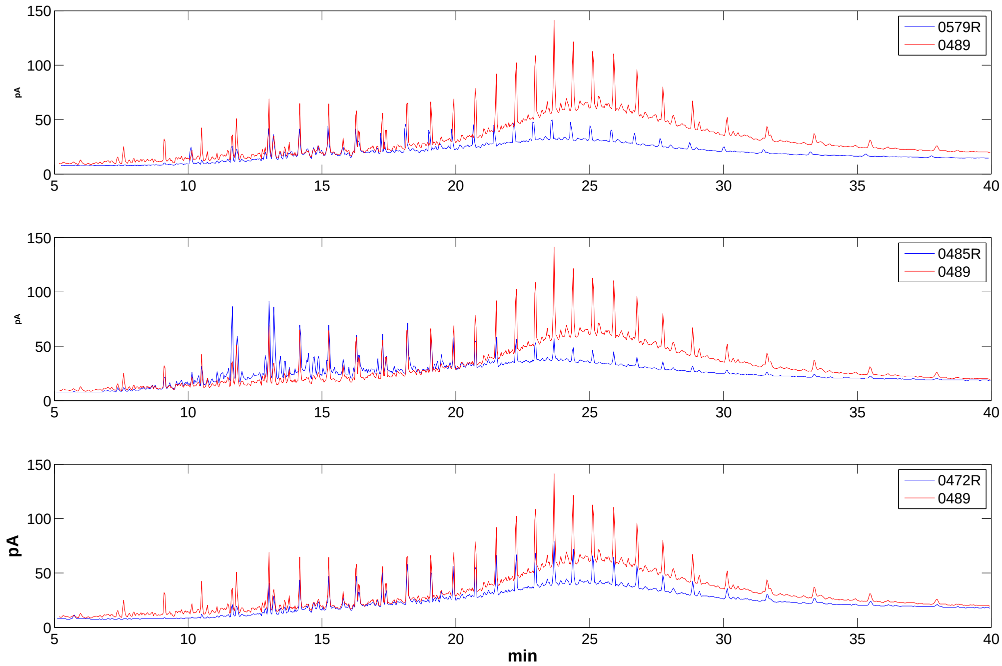

Figure A.8: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0489) and the reference samples.

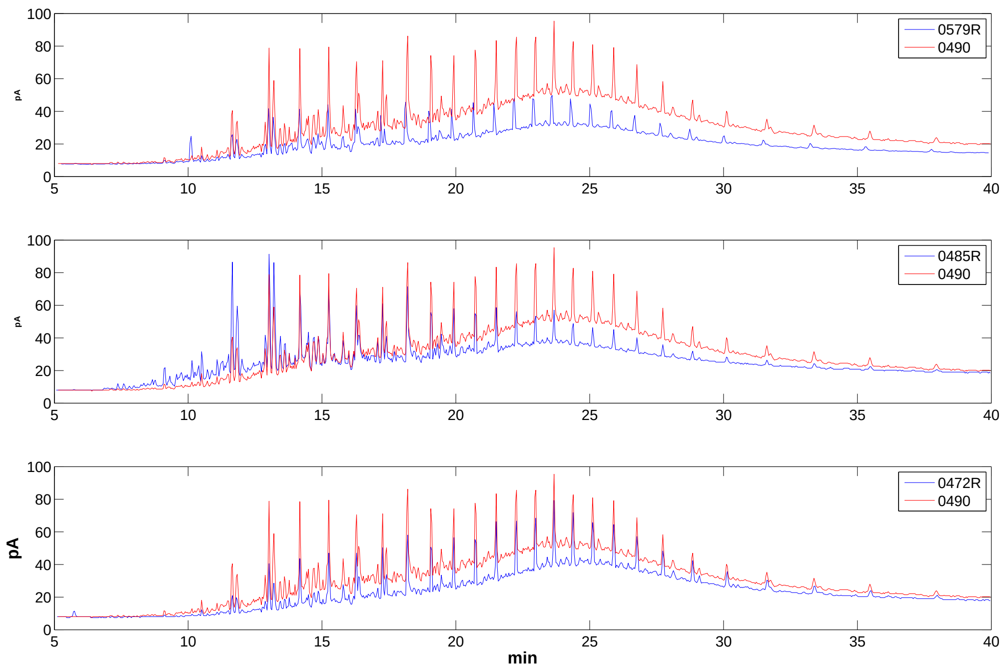

Figure A.9: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0490) and the reference samples.

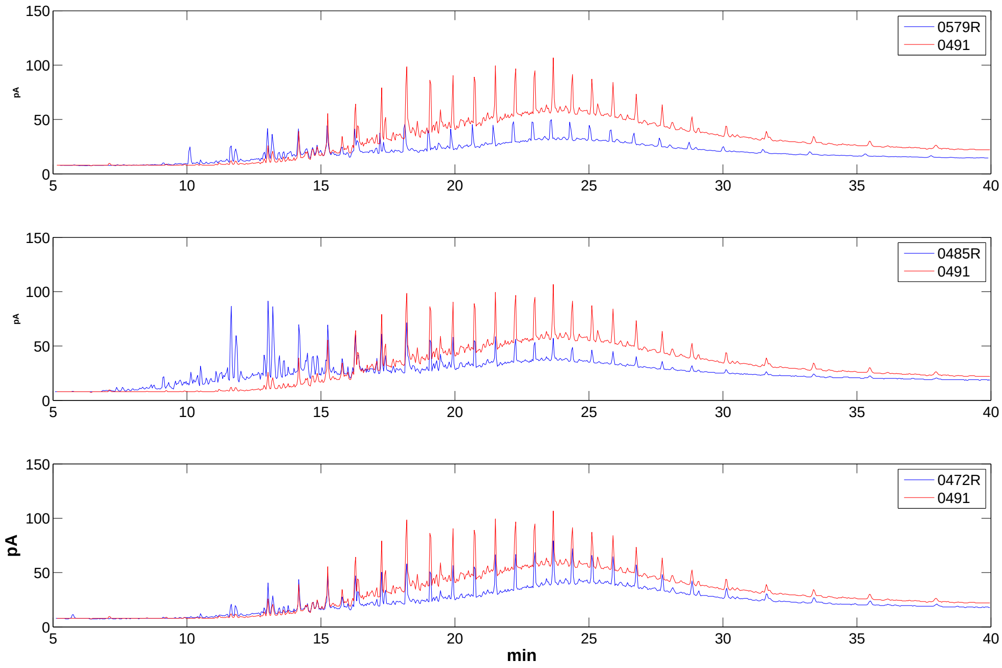

Figure A.10: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0491) and the reference samples.

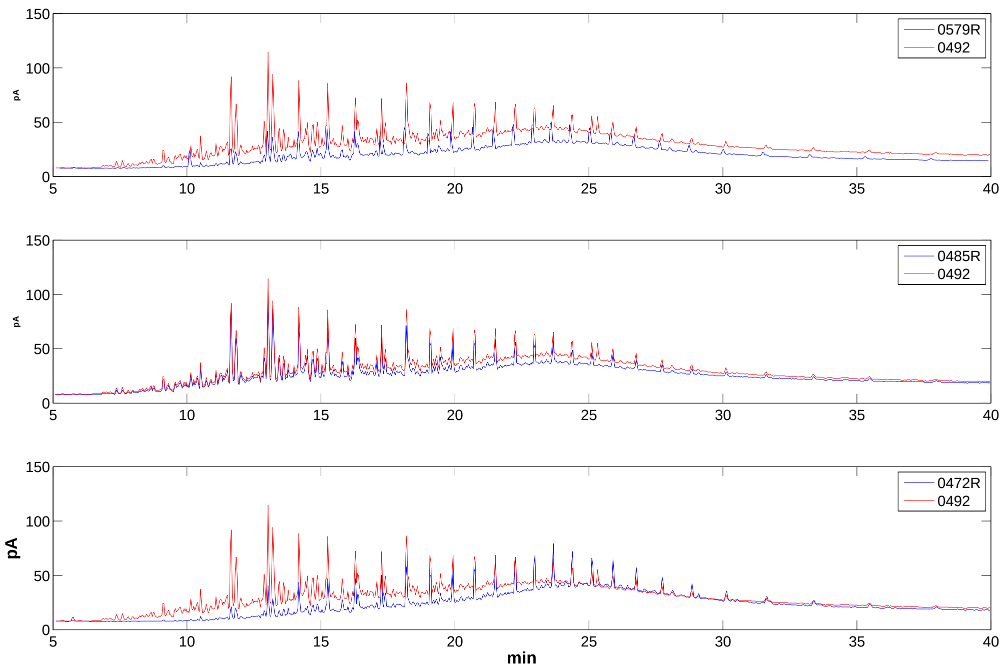

Figure A.11: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0492) and the reference samples.

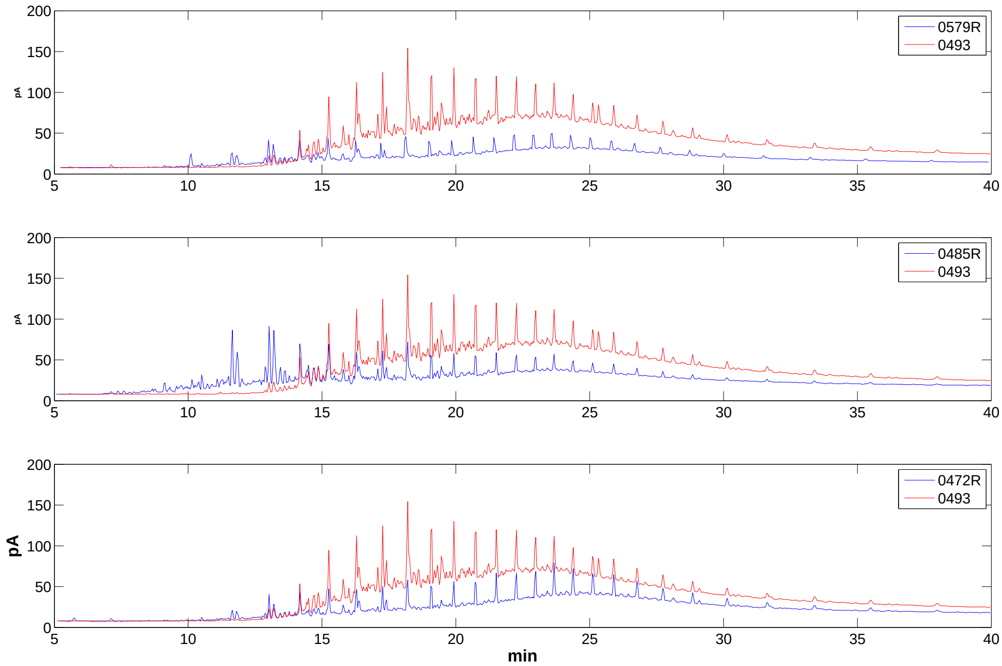

Figure A.12: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0493) and the reference samples.

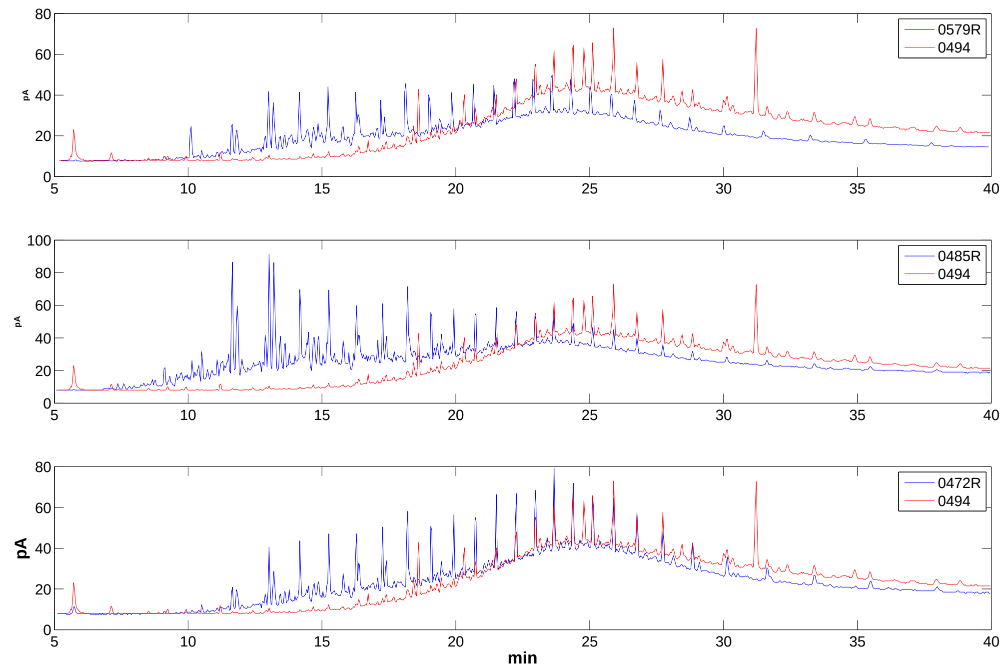

Figure A.13: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0494) and the reference samples.

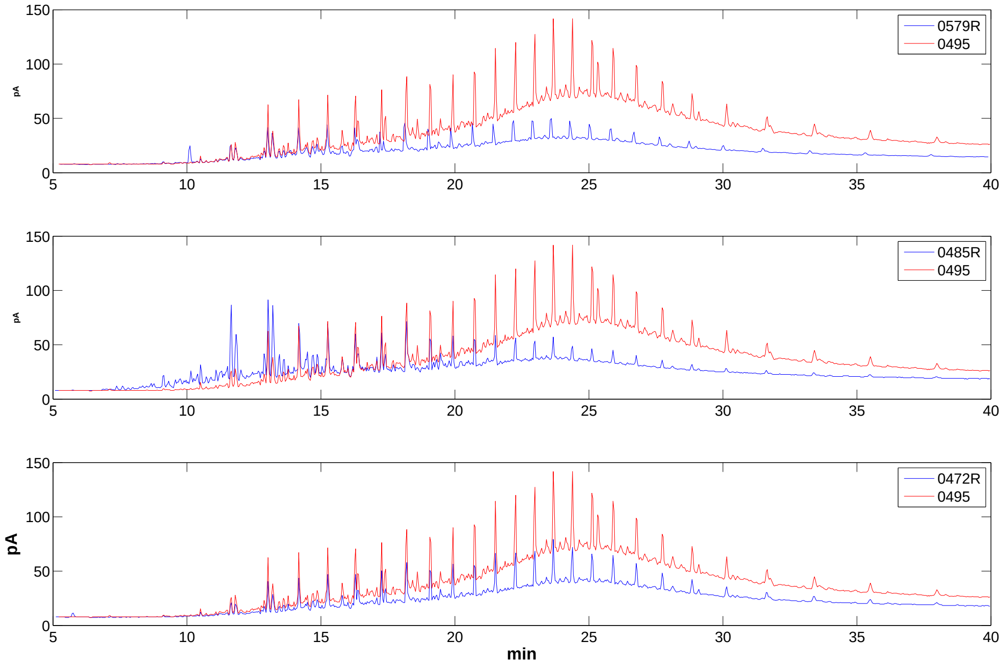

Figure A.14: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0495) and the reference samples.

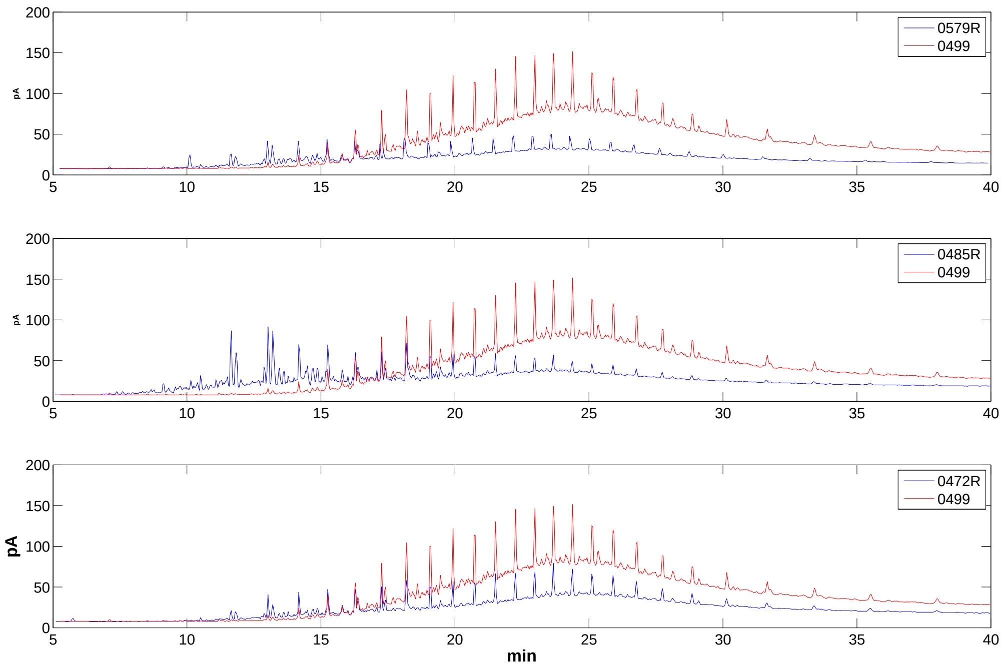

Figure A.15: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0499) and the reference samples.

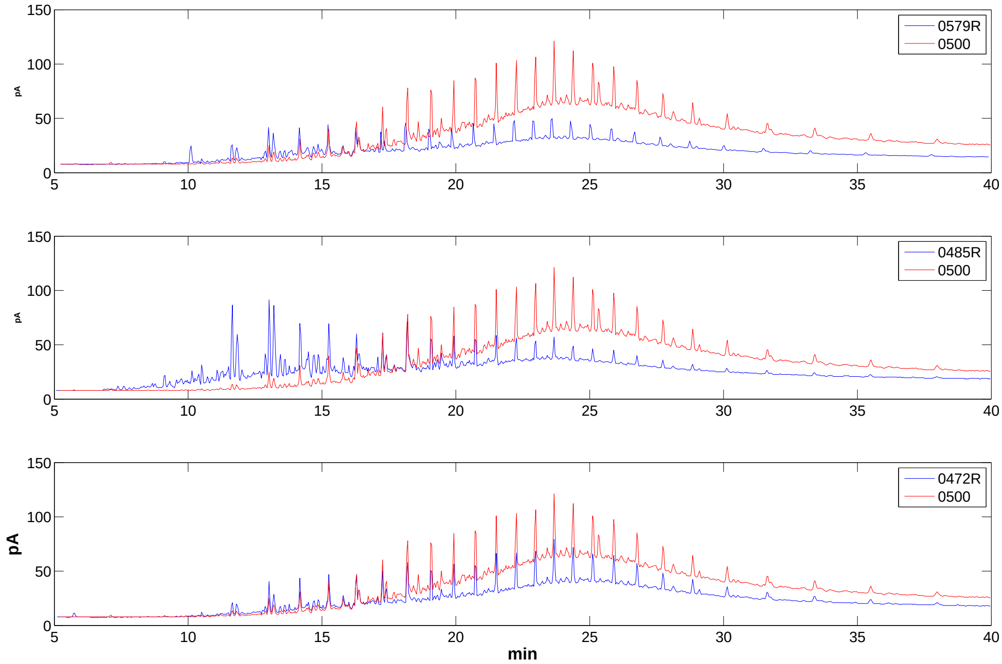

Figure A.16: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0500) and the reference samples.

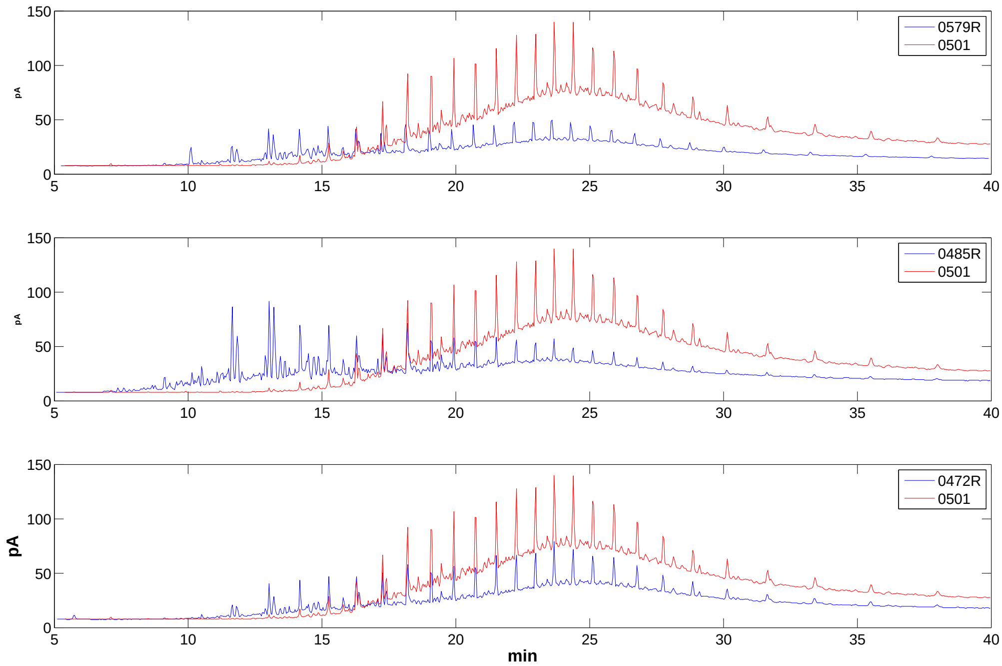

Figure A.17: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0501) and the reference samples.

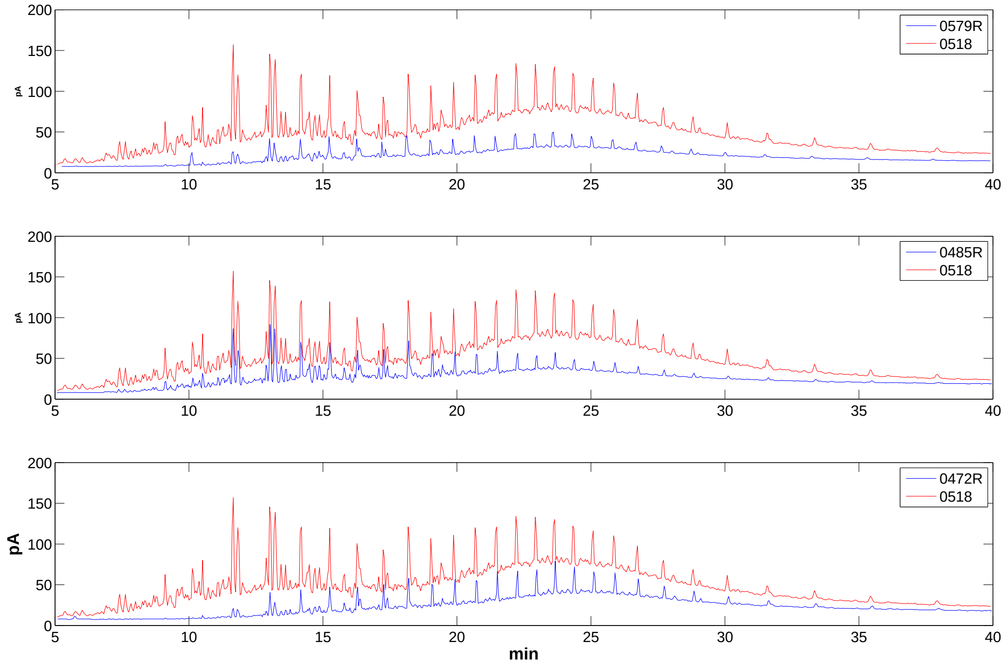

Figure A.18: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0518) and the reference samples.

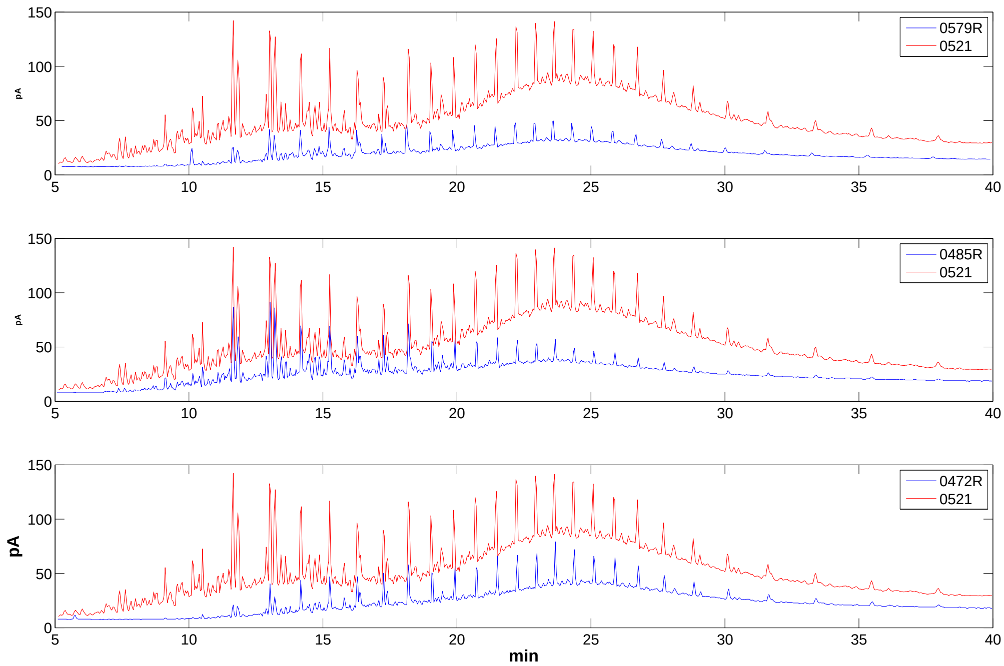

Figure A.19: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0521) and the reference samples.

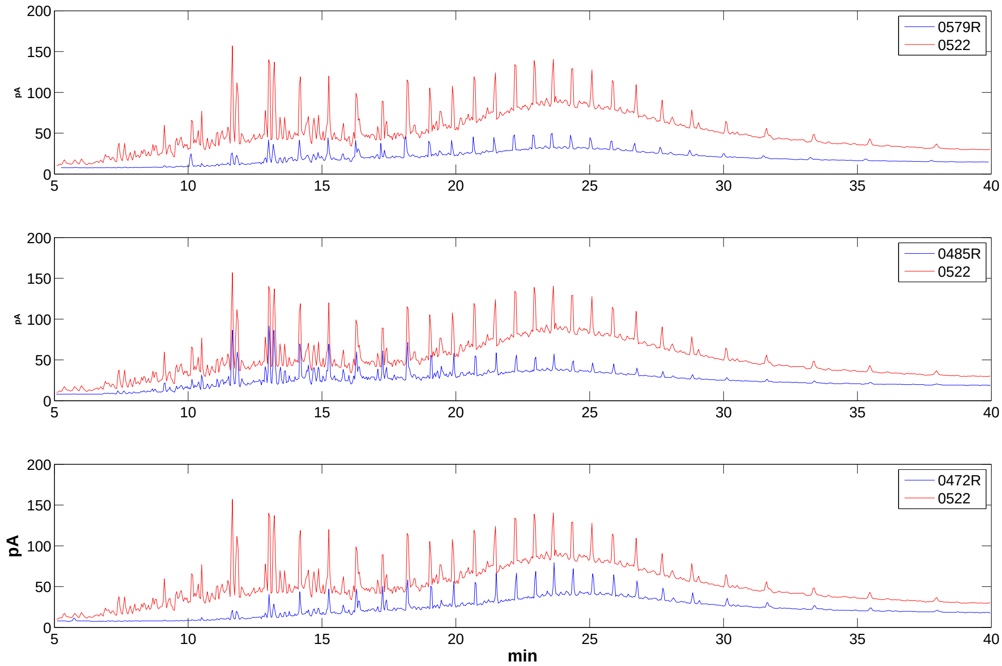

Figure A.20: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0522) and the reference samples.

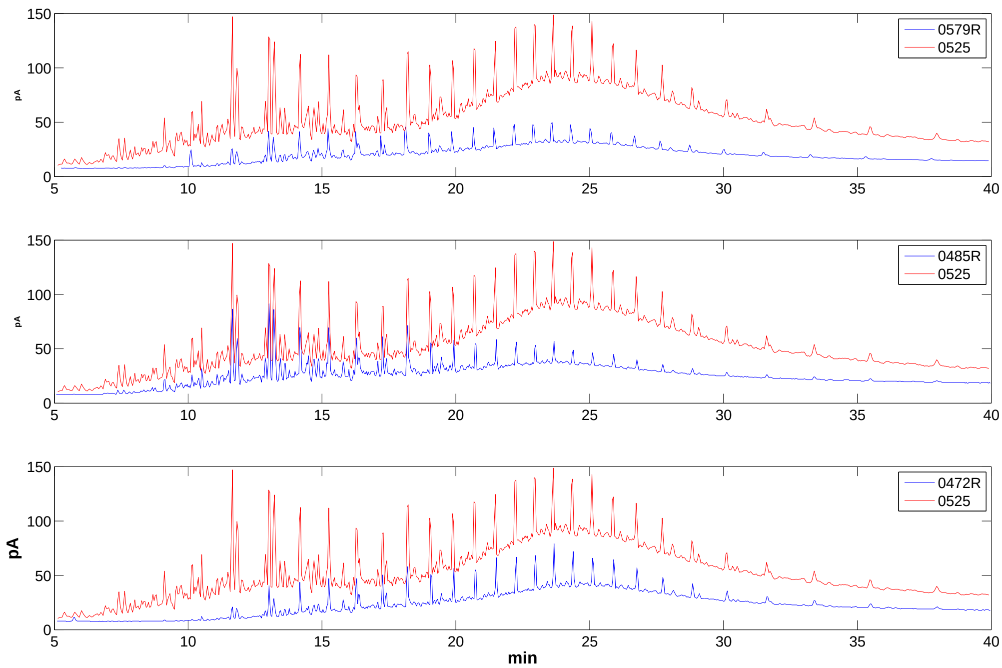

Figure A.21: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0525) and the reference samples.

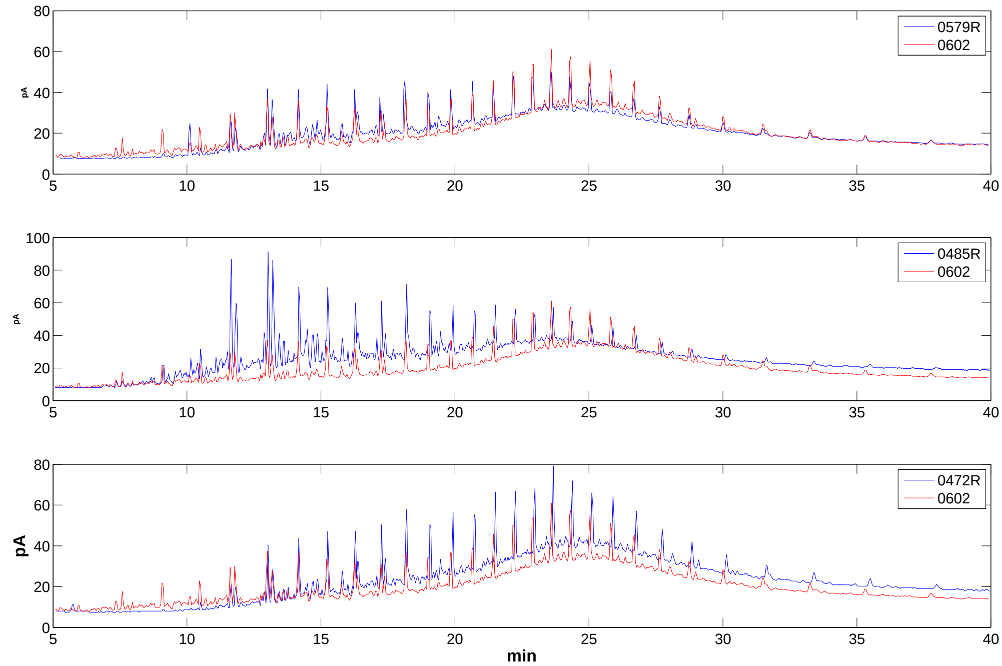

Figure A.22: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0602) and the reference samples.

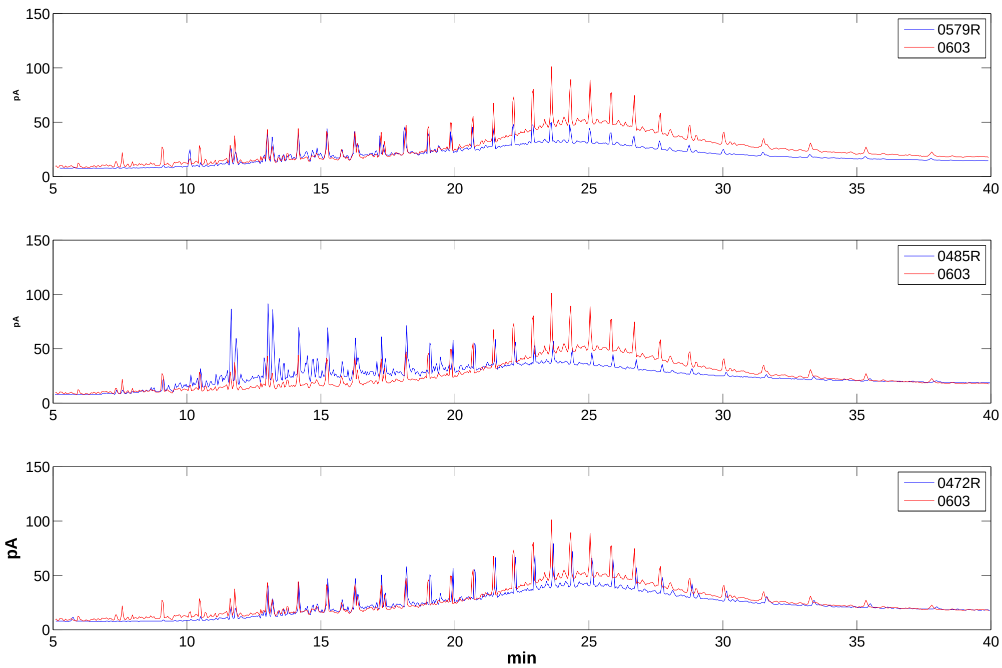

Figure A.23: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0603) and the reference samples.

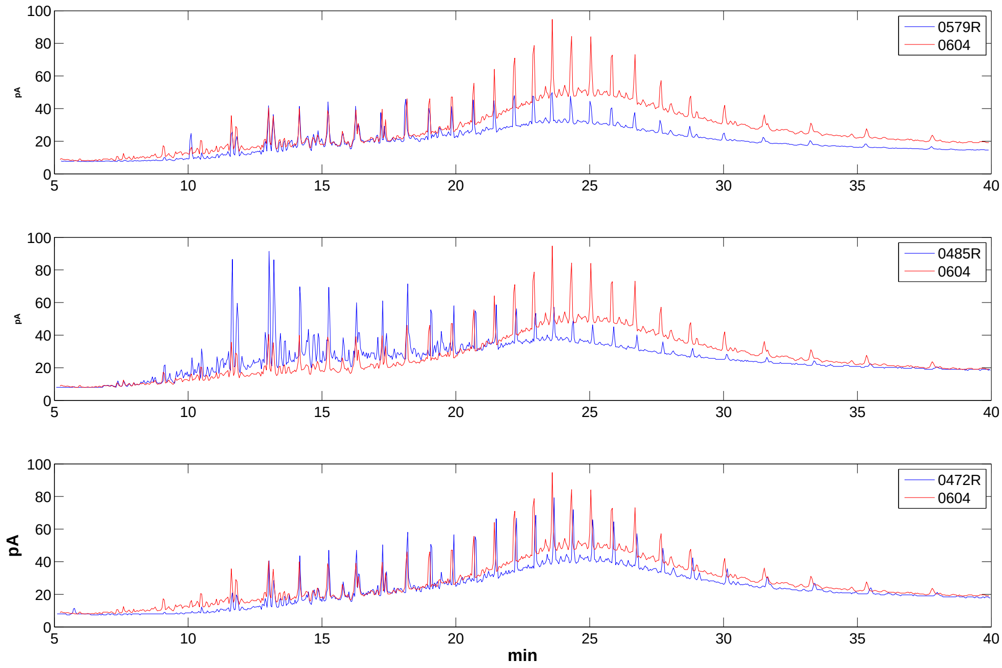

Figure A.24: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0604) and the reference samples.

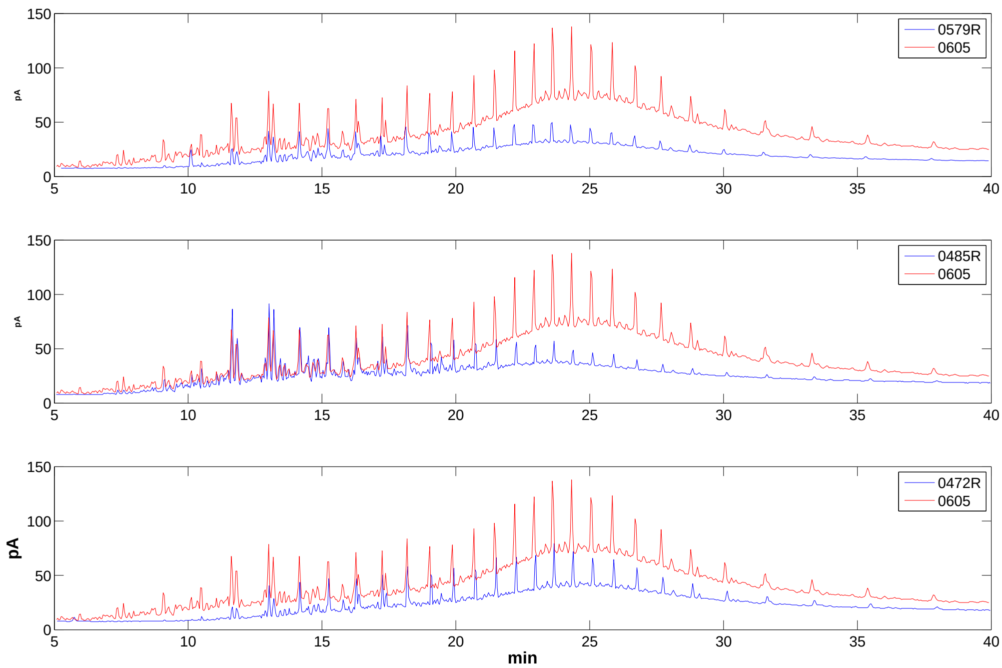

Figure A.25: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0605) and the reference samples.

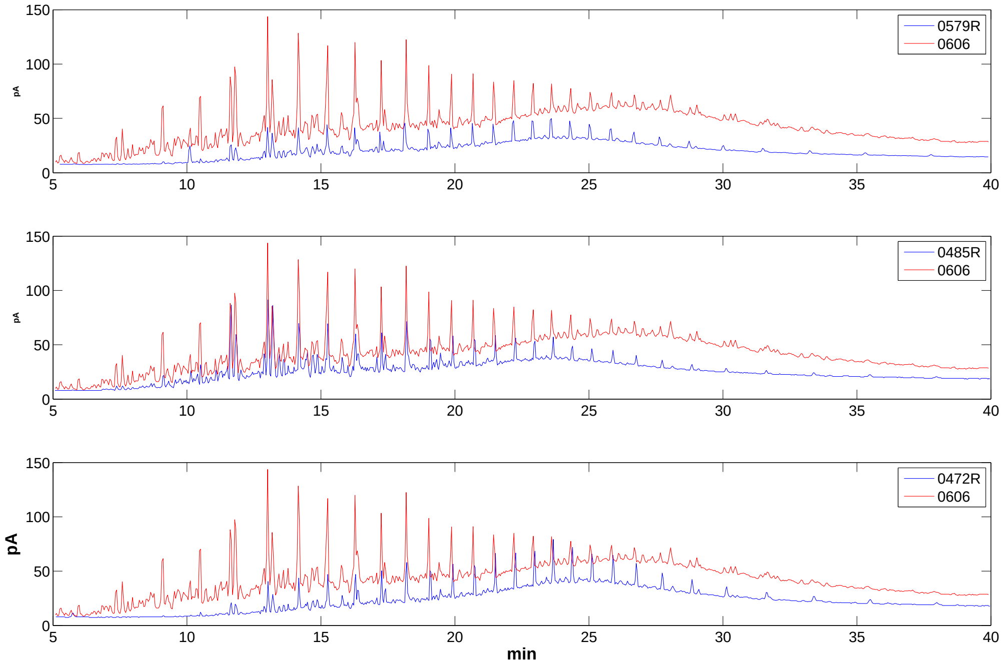

Figure A.26: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0606) and the reference samples.

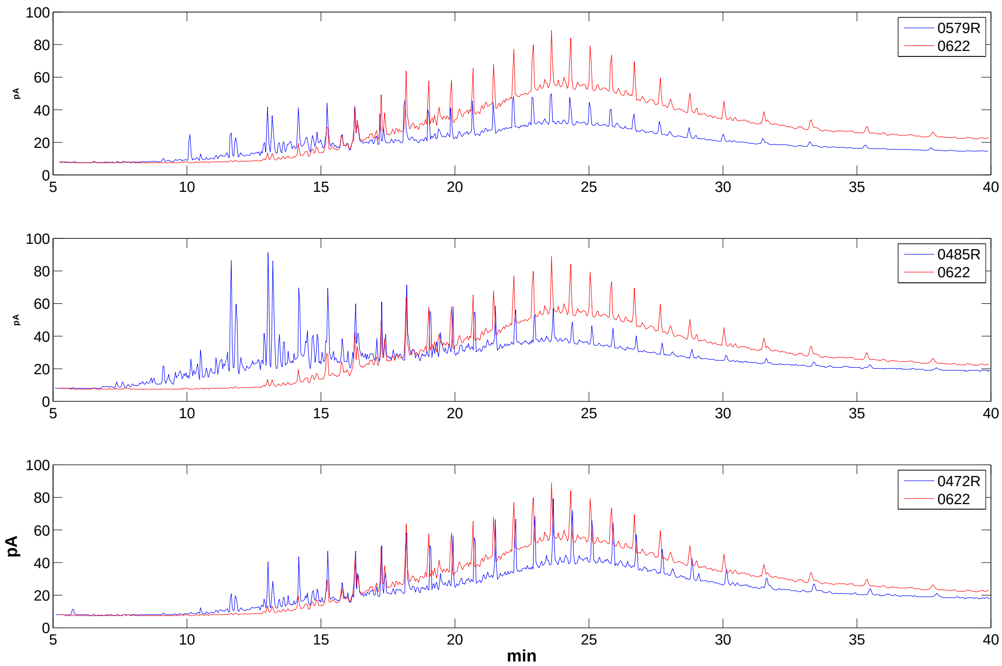

Figure A.27: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0622) and the reference samples.

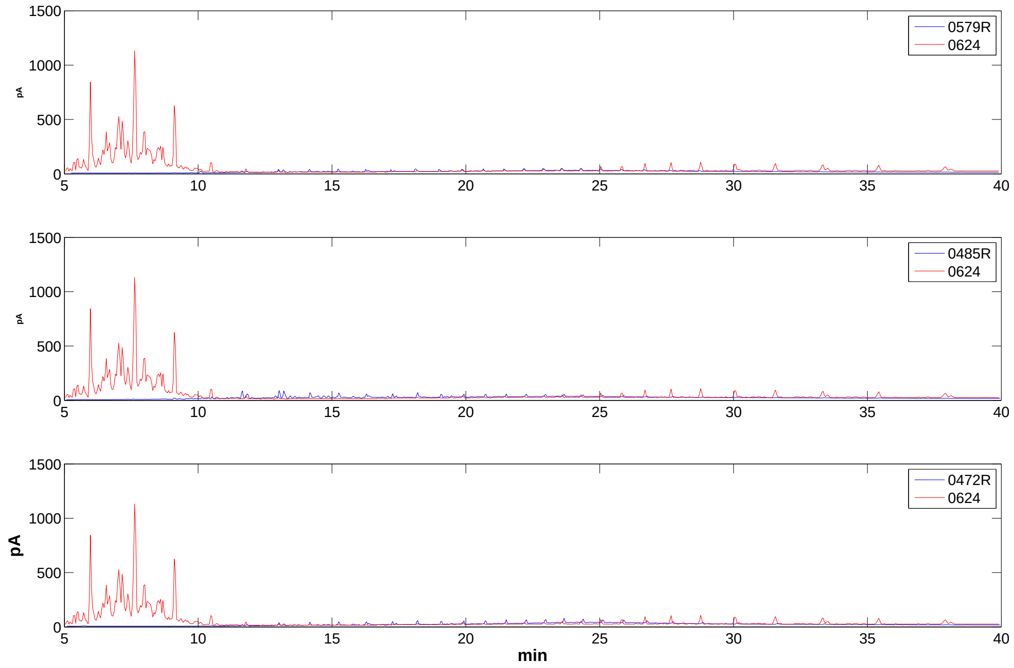

Figure A.28: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0624) and the reference samples.

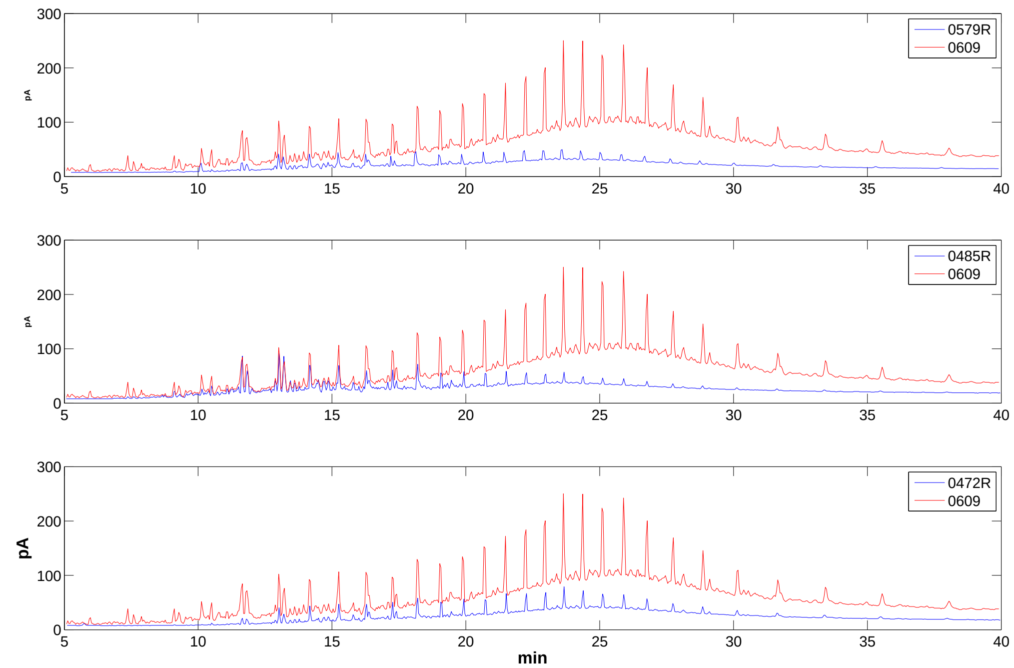

Figure A.29: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0609) and the reference samples.

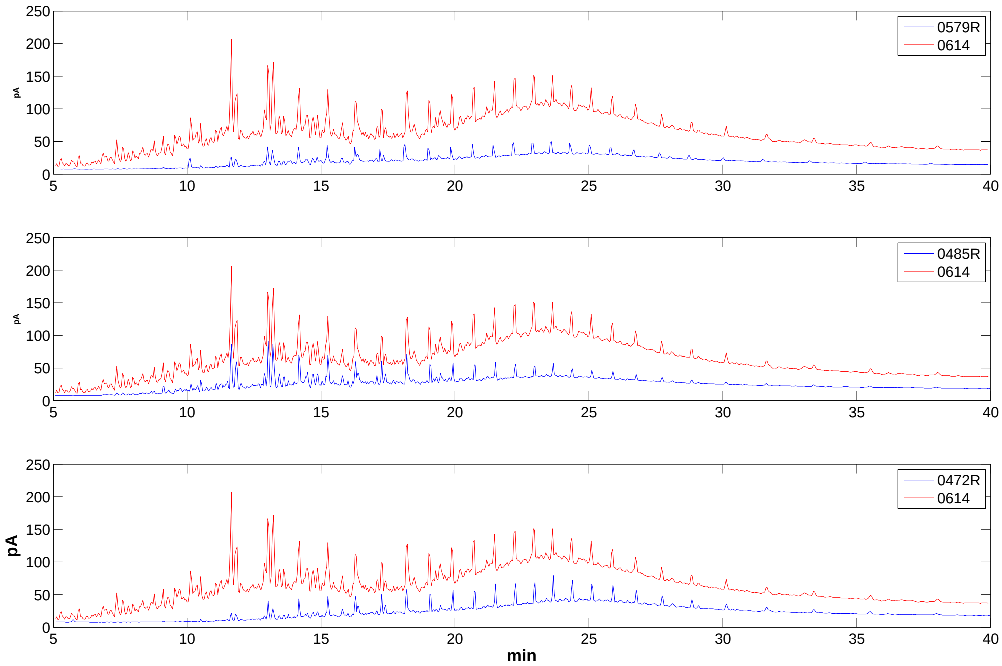

Figure A.30: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0614) and the reference samples.

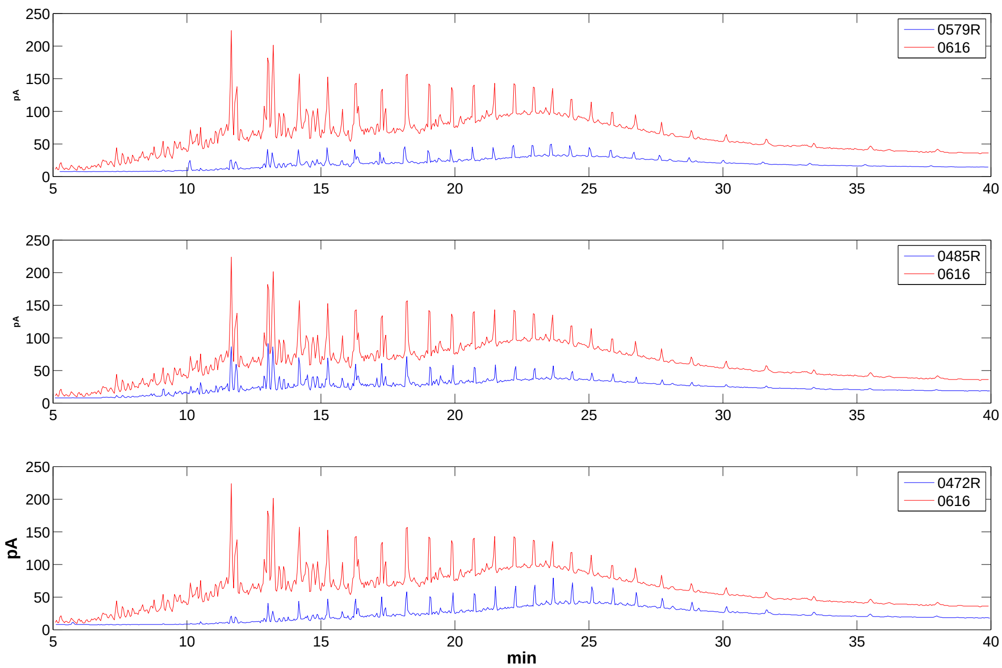

Figure A.31: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0616) and the reference samples.

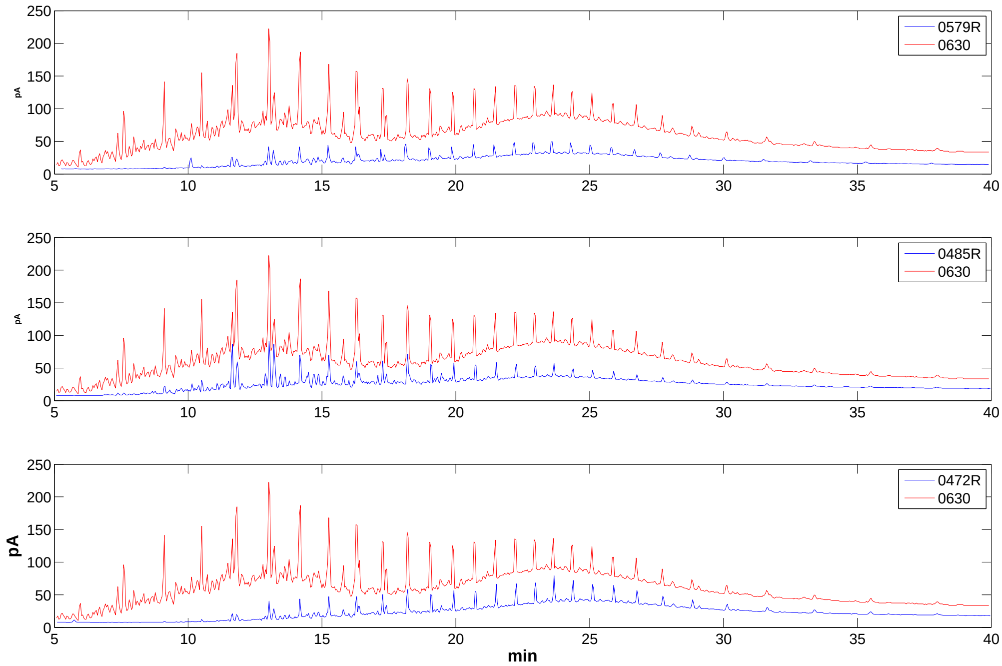

Figure A.32: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0630) and the reference samples.

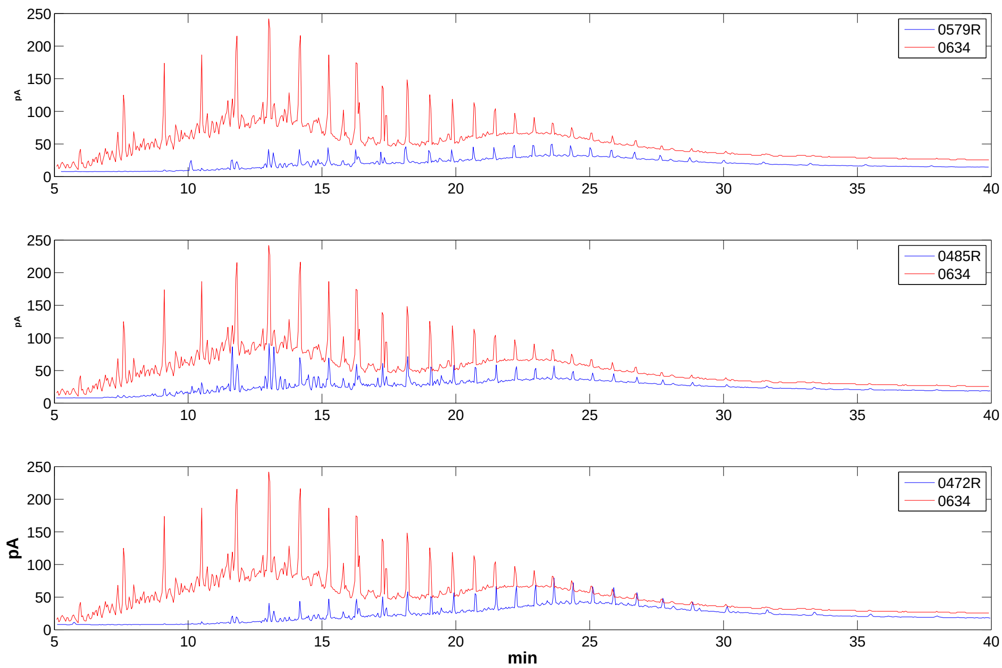

Figure A.33: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0634) and the reference samples.

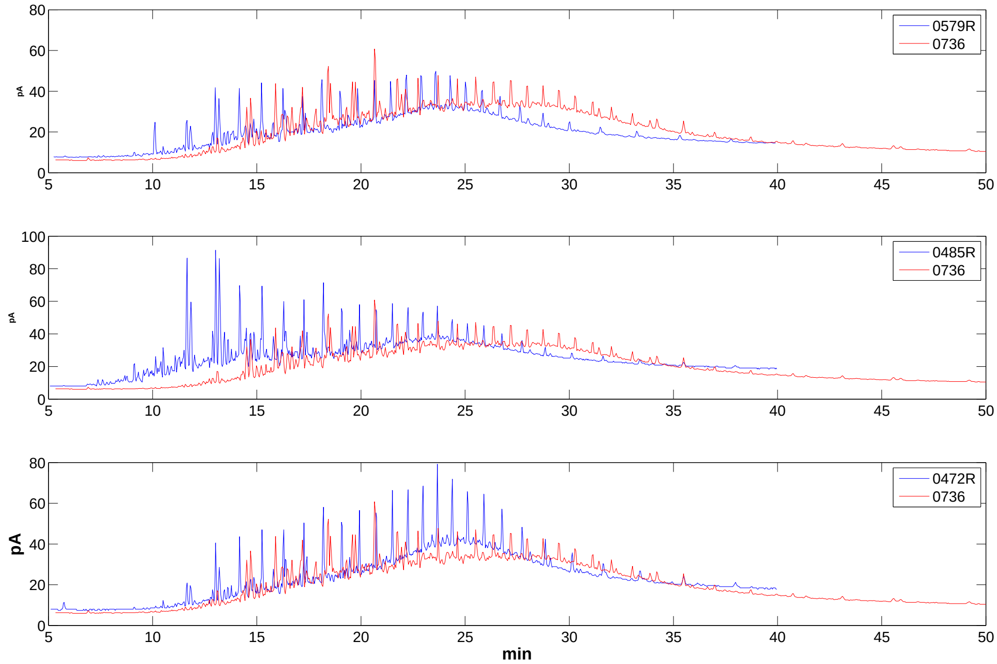

Figure A.34: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0736) and the reference samples.

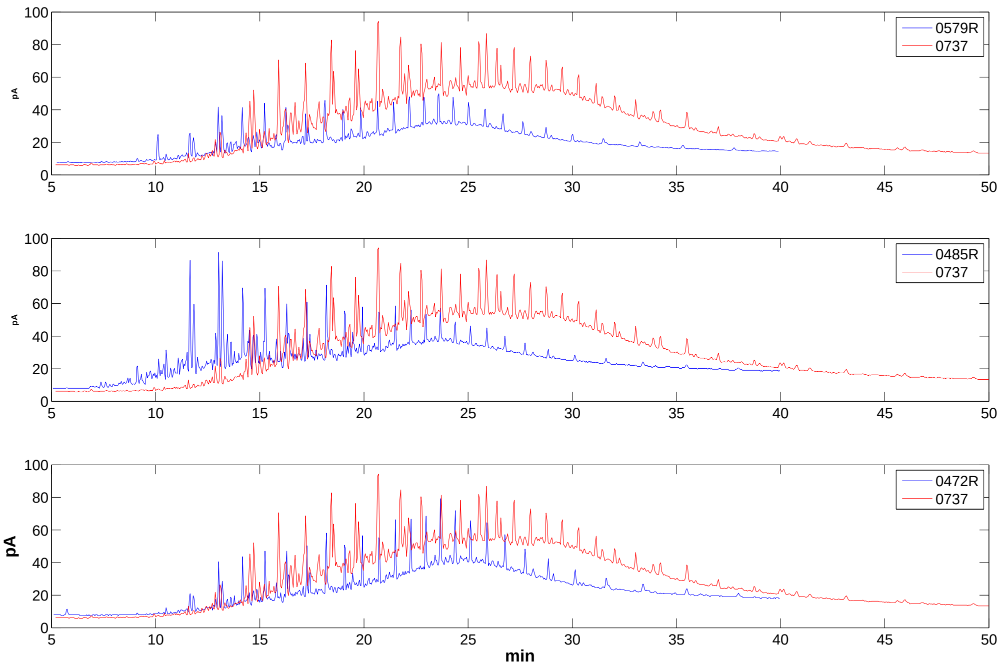

Figure A.35: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0737) and the reference samples.

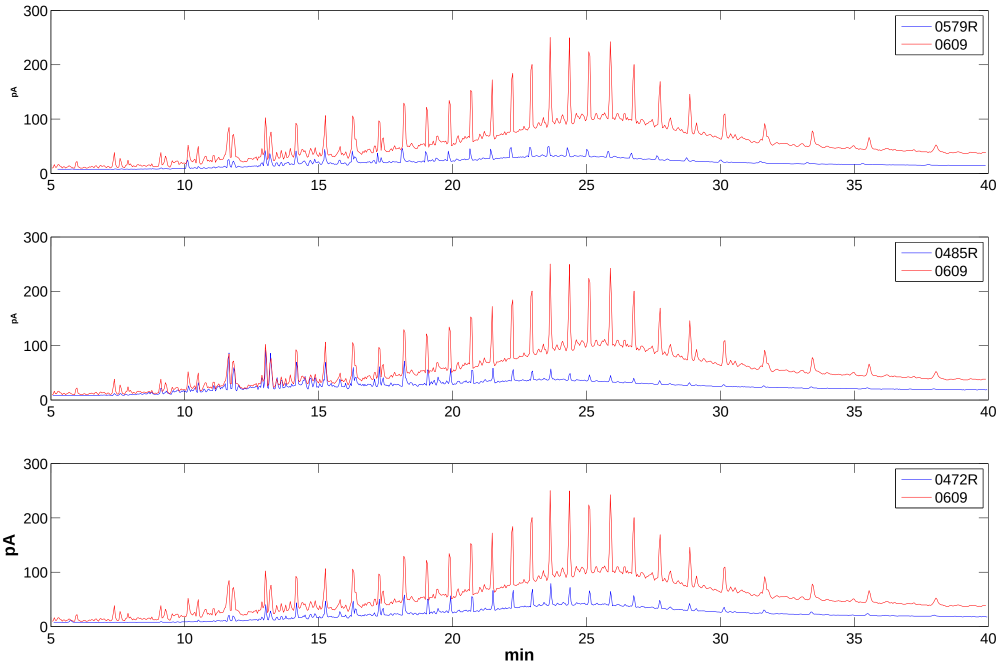

Figure A.36: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2009-0609) and the reference samples.

B

CEN LEVEL I - GC/FID VISUAL INSPECTION: "SERVER" CASE

For "Server" case, based on GC/FID analysis result done by SINTEF [Almås et al., 2007], which was available in form of figures in pdf file (no digital data available), the author digitized all GC/FID chromatogram of the samples by mean of graph digitizing software, *windig25*. Afterward, Level 1 screening by overlaying the chromatogram of the spill sample on top of the reference sample could be easily performed in Matlab. The results are presented in this appendix.

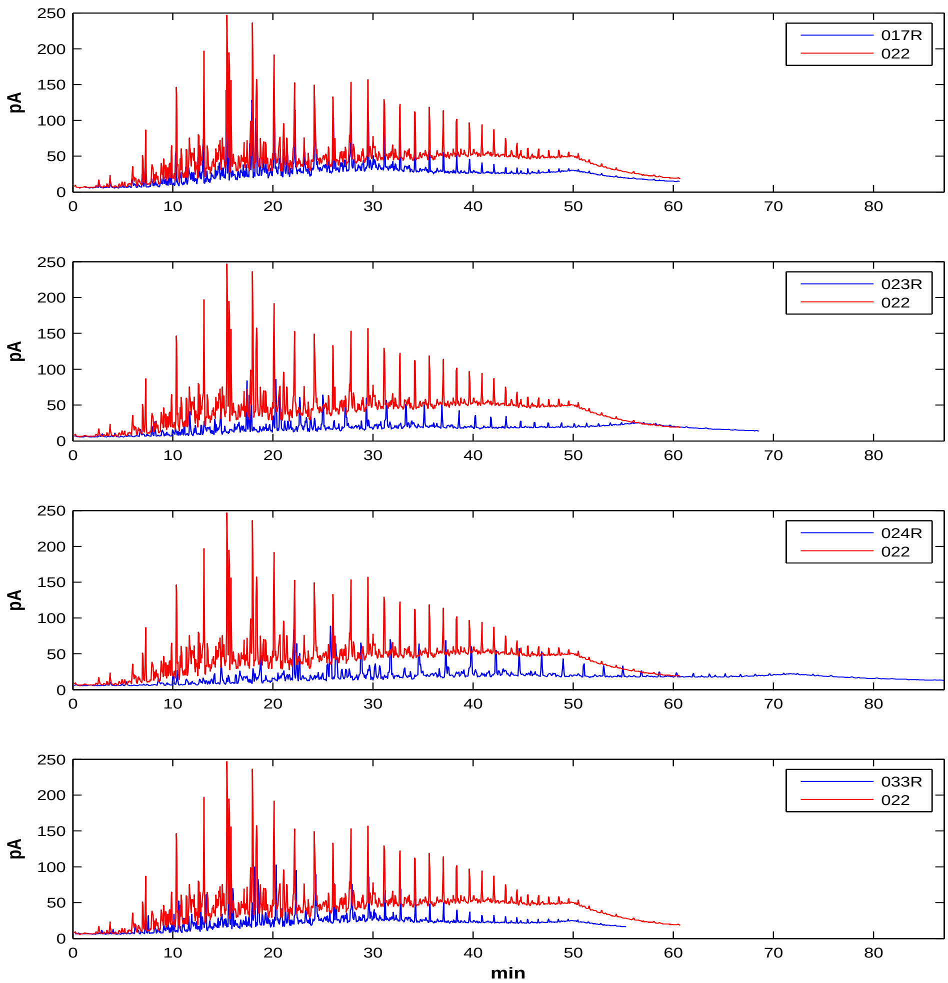

Figure B.1: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0022) and the reference samples.

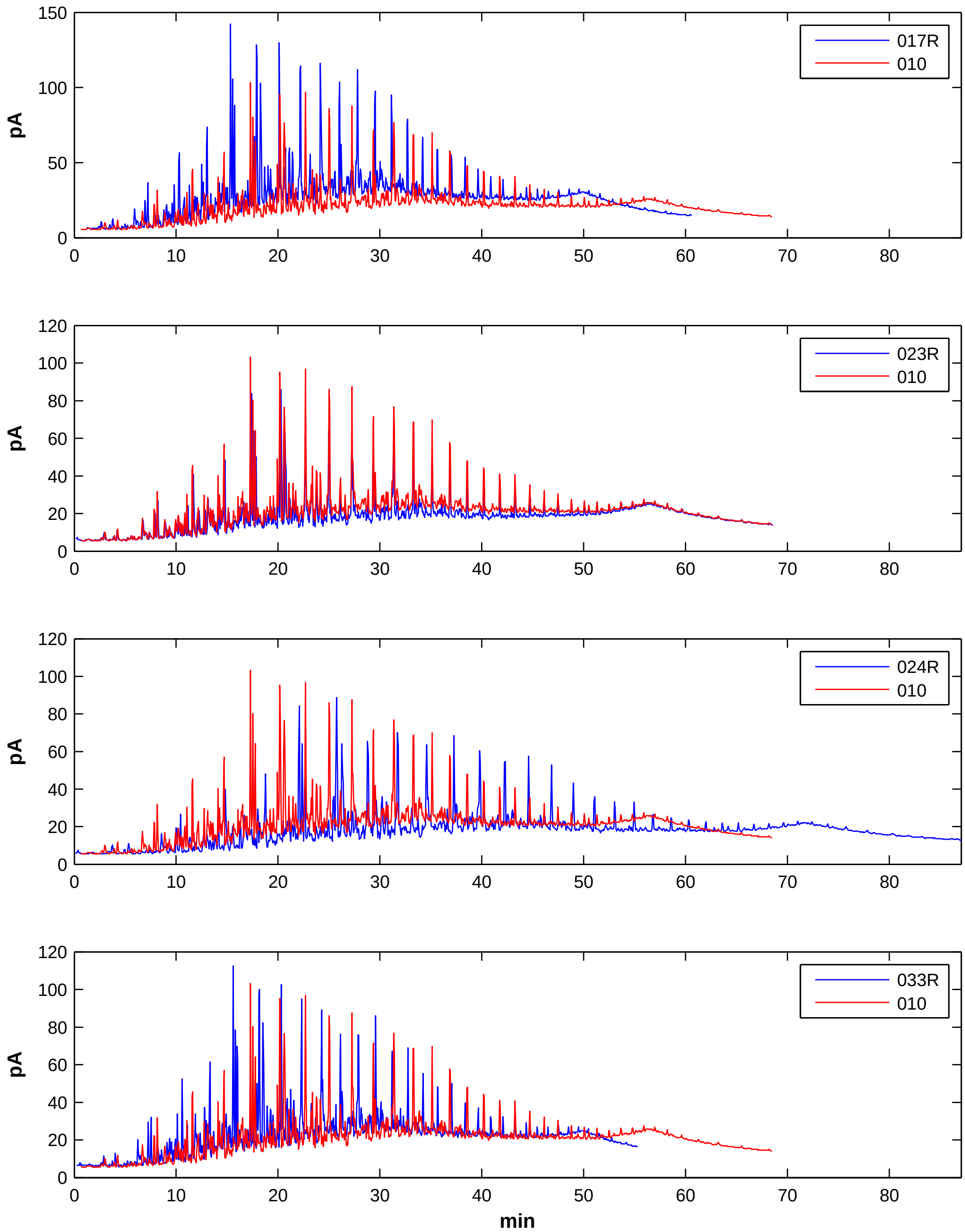

Figure B.2: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0010) and the reference samples.

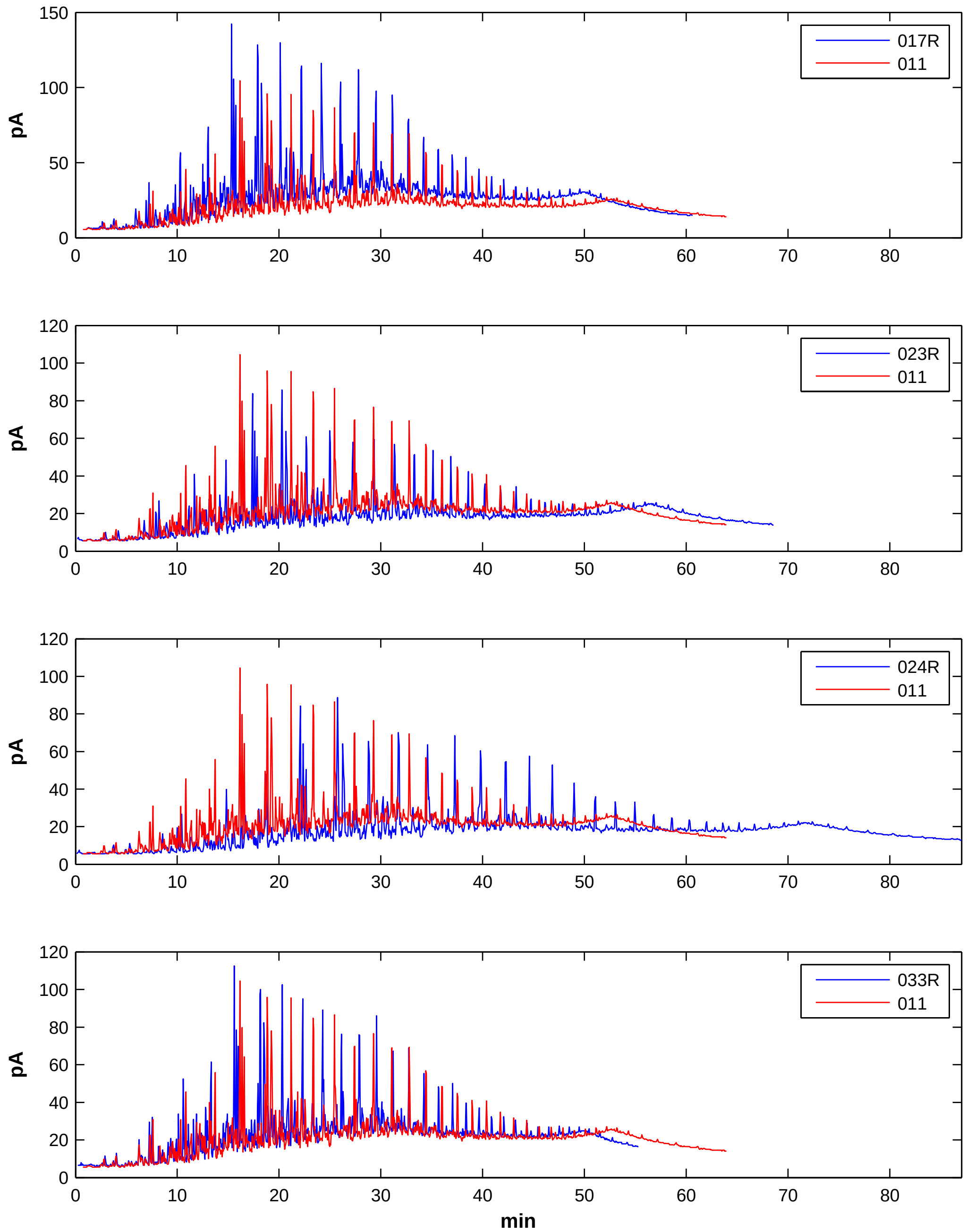

Figure B.3: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0011) and the reference samples.

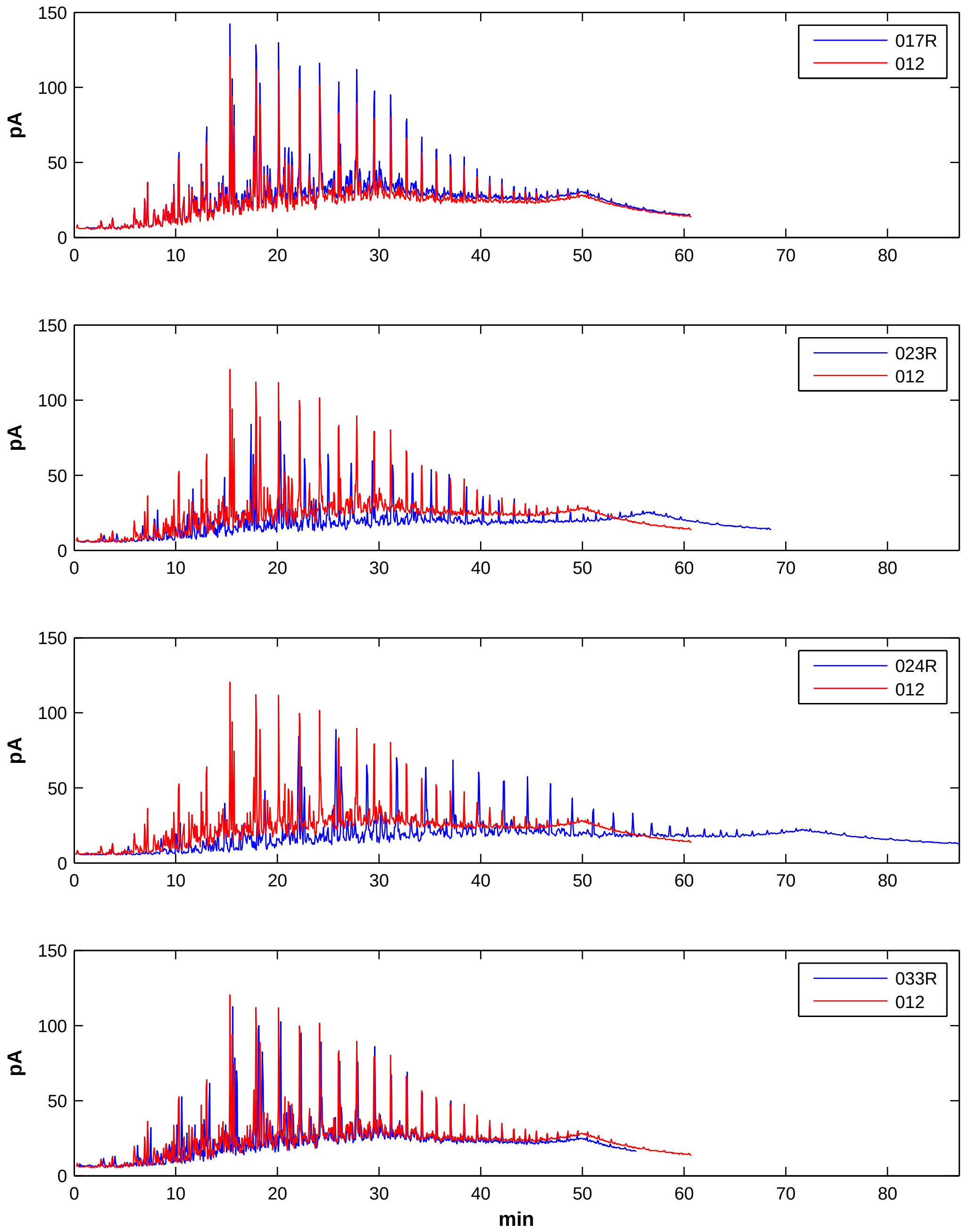

Figure B.4: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0012) and the reference samples.

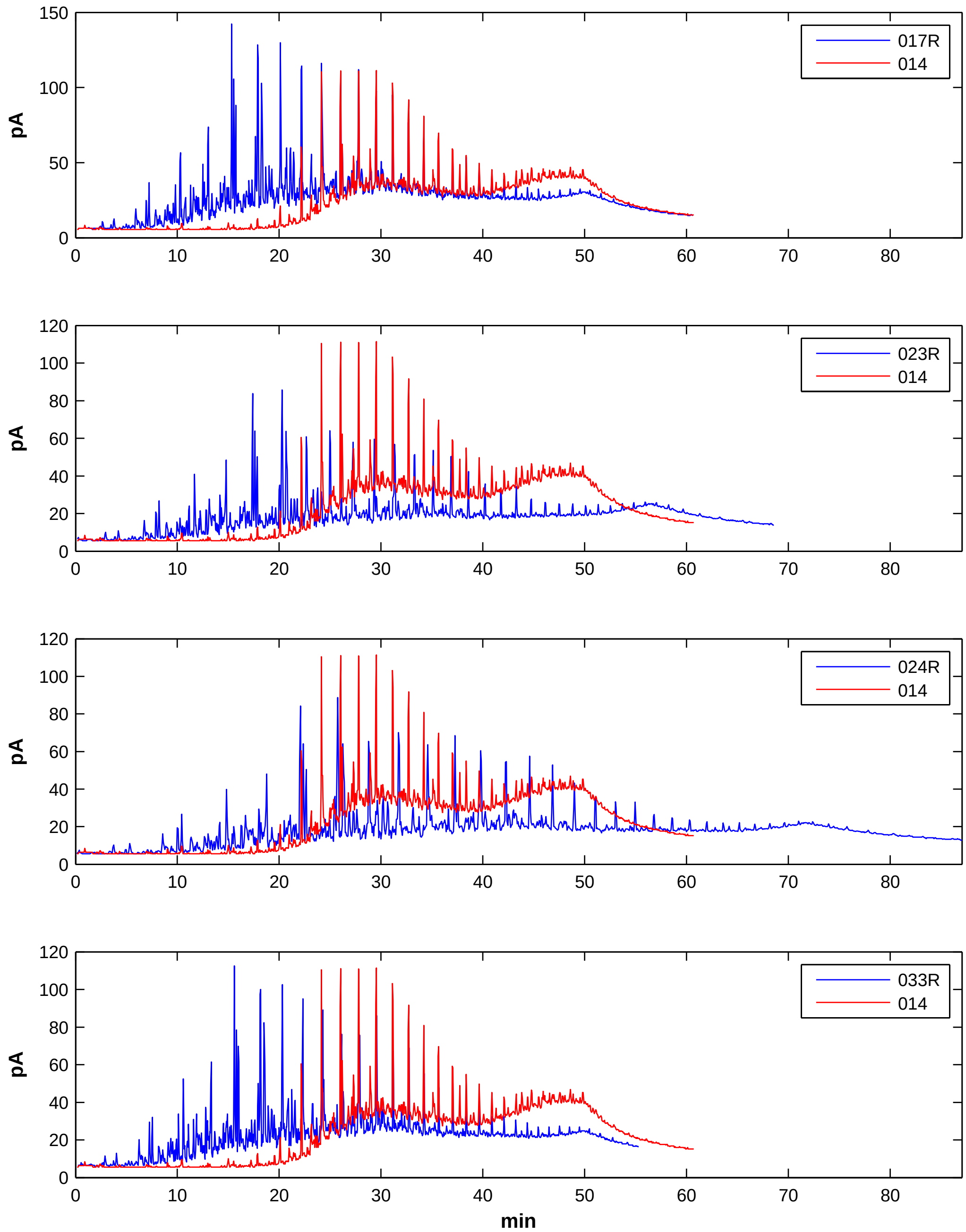

Figure B.5: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0014) and the reference samples.

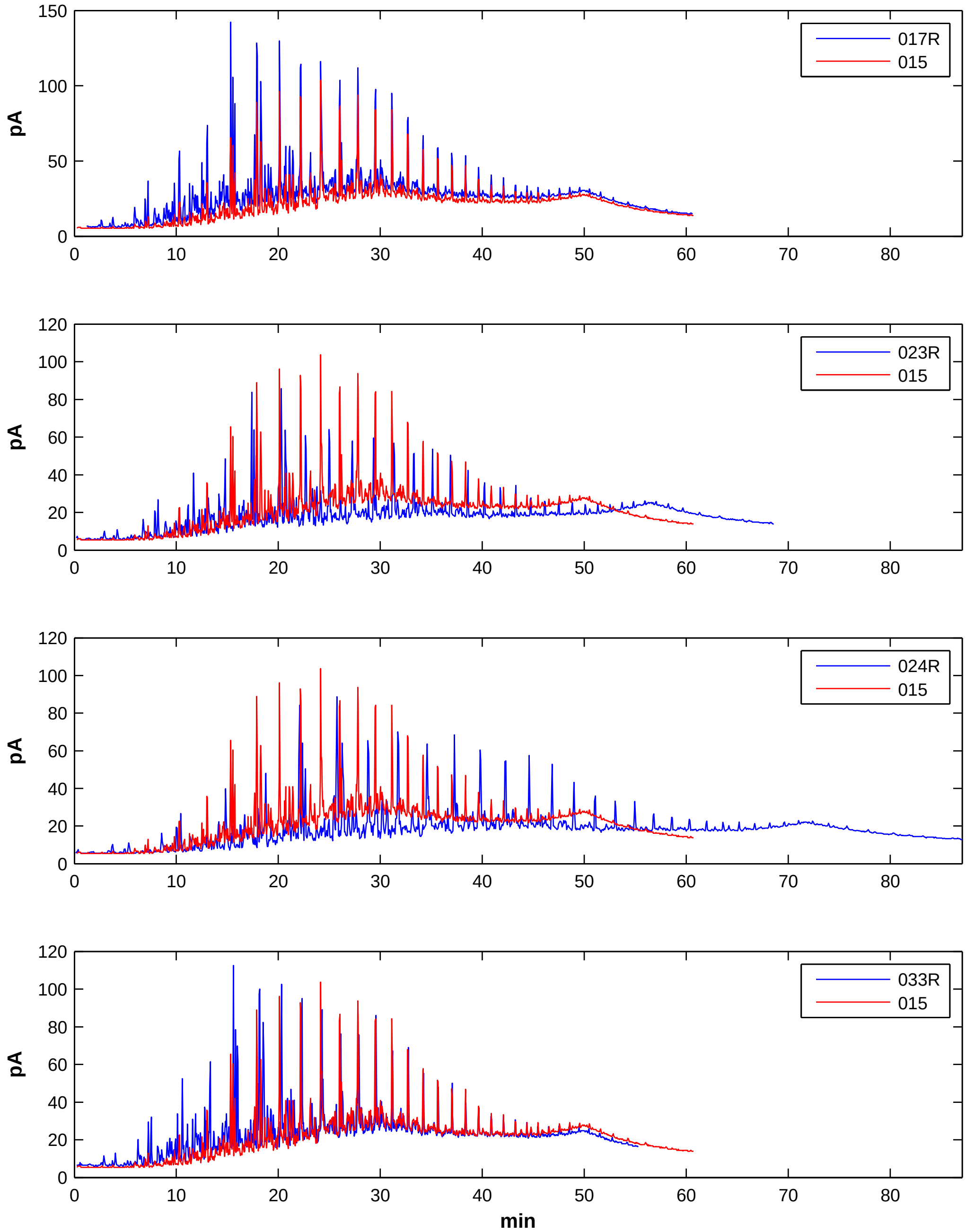

Figure B.6: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0015) and the reference samples.

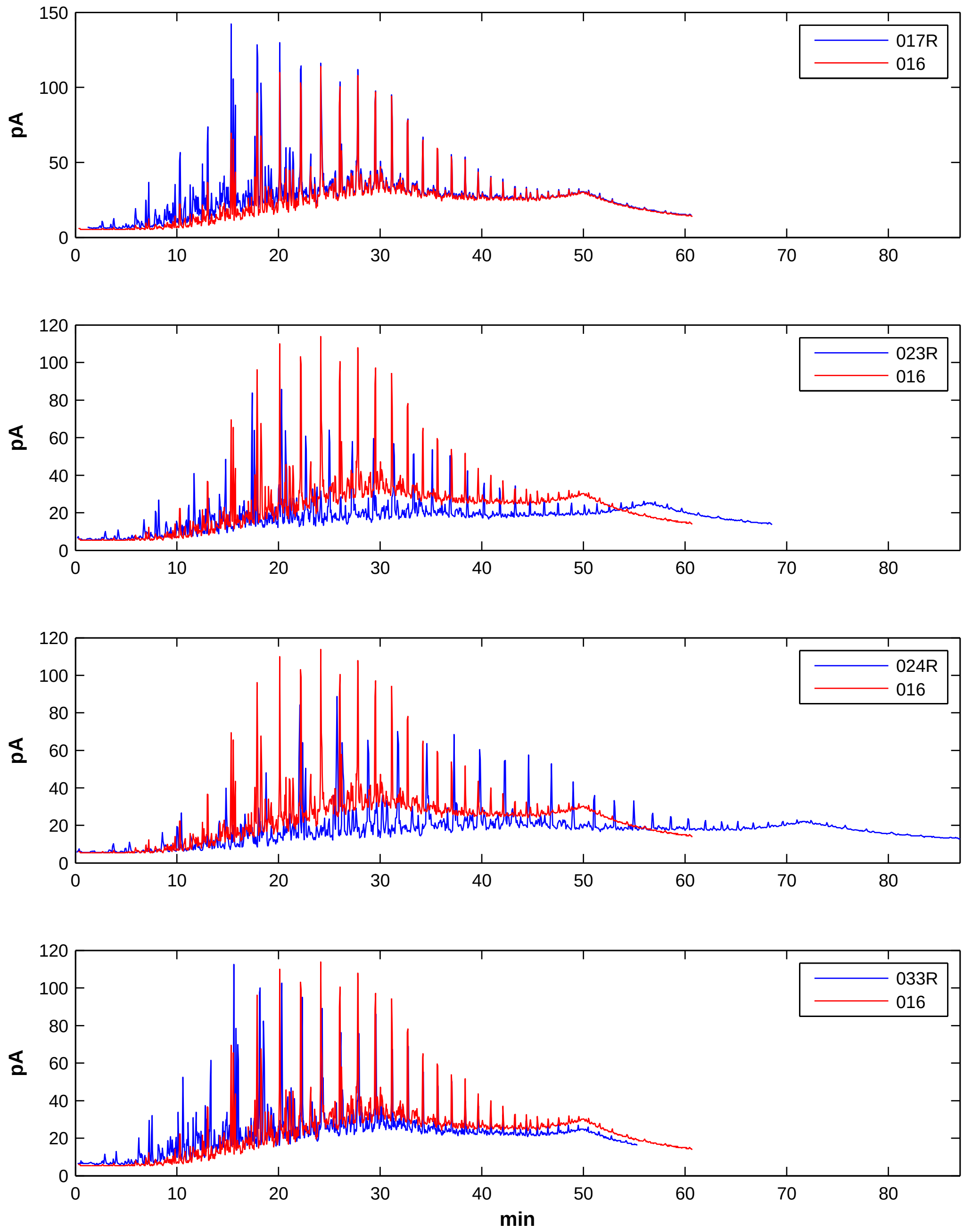

Figure B.7: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0016) and the reference samples.

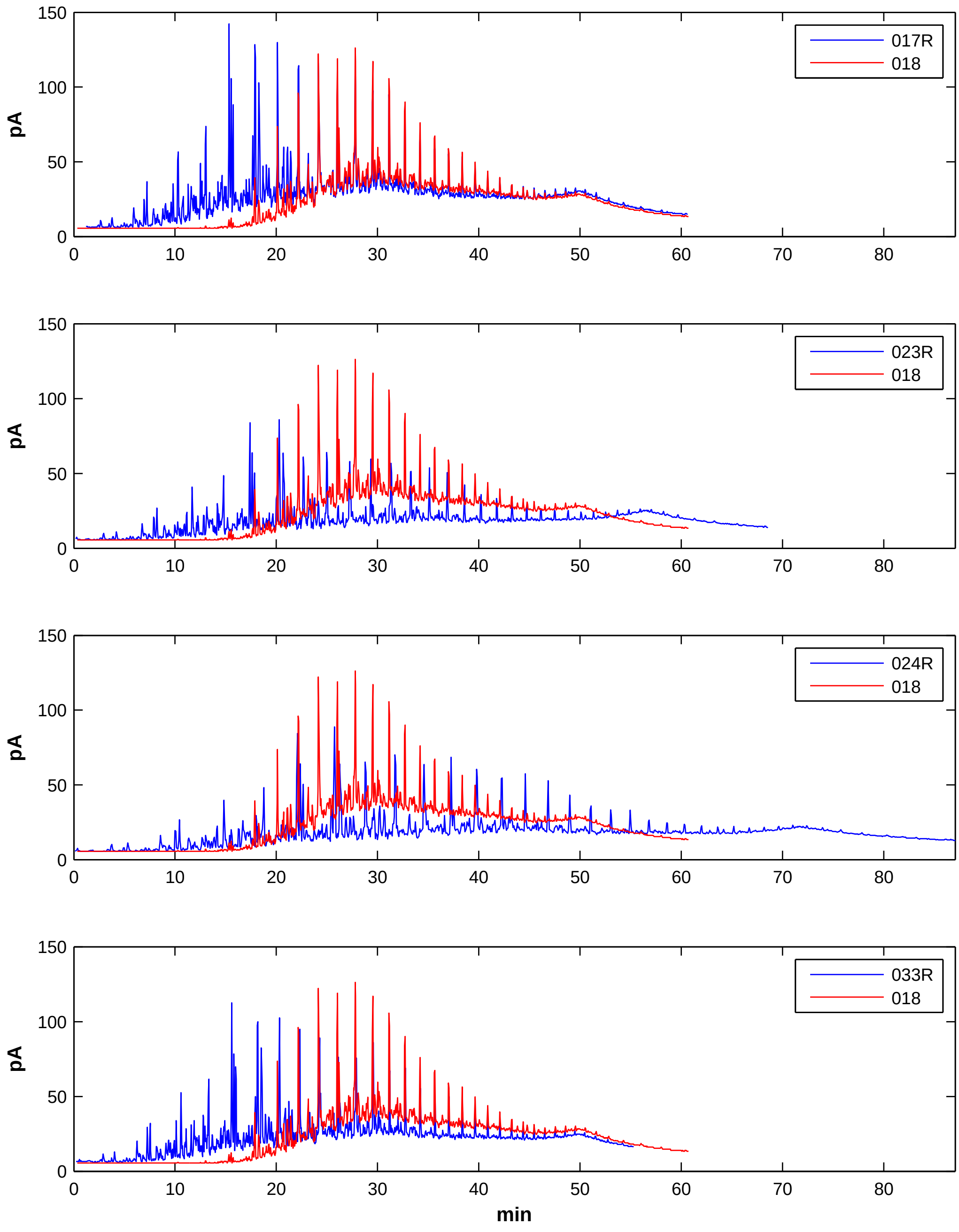

Figure B.8: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0018) and the reference samples.

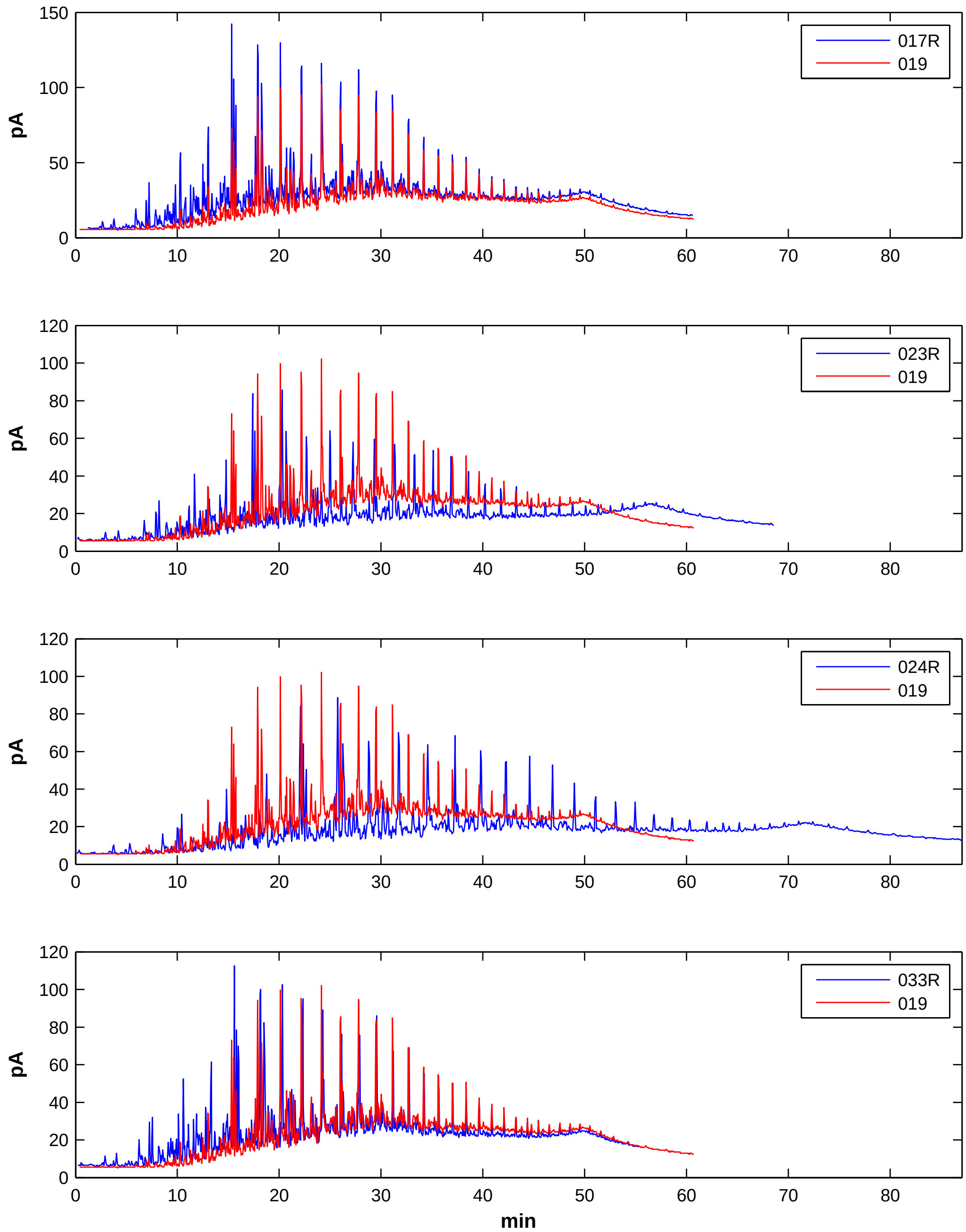

Figure B.9: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0019) and the reference samples.

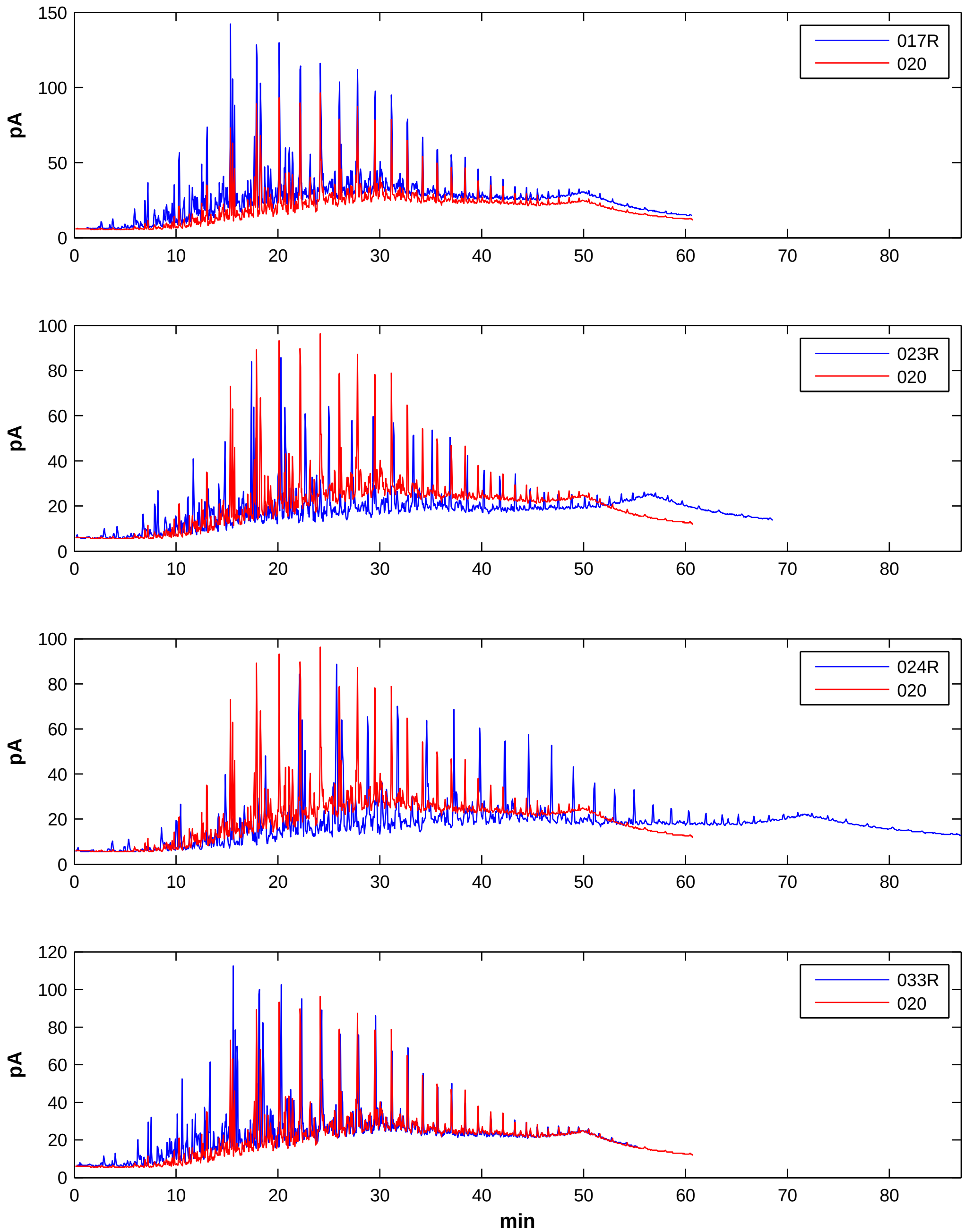

Figure B.10: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0020) and the reference samples.

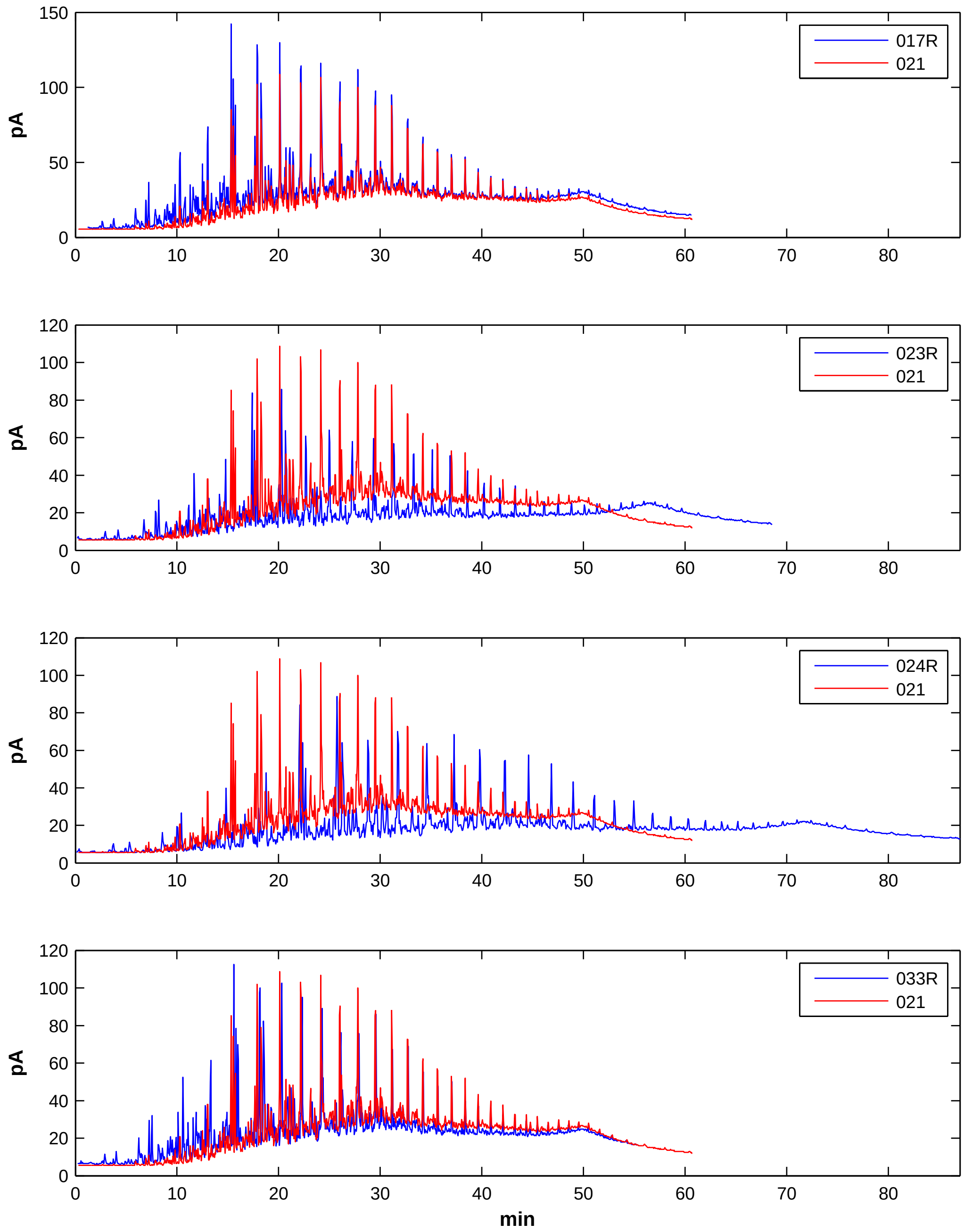

Figure B.11: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0021) and the reference samples.

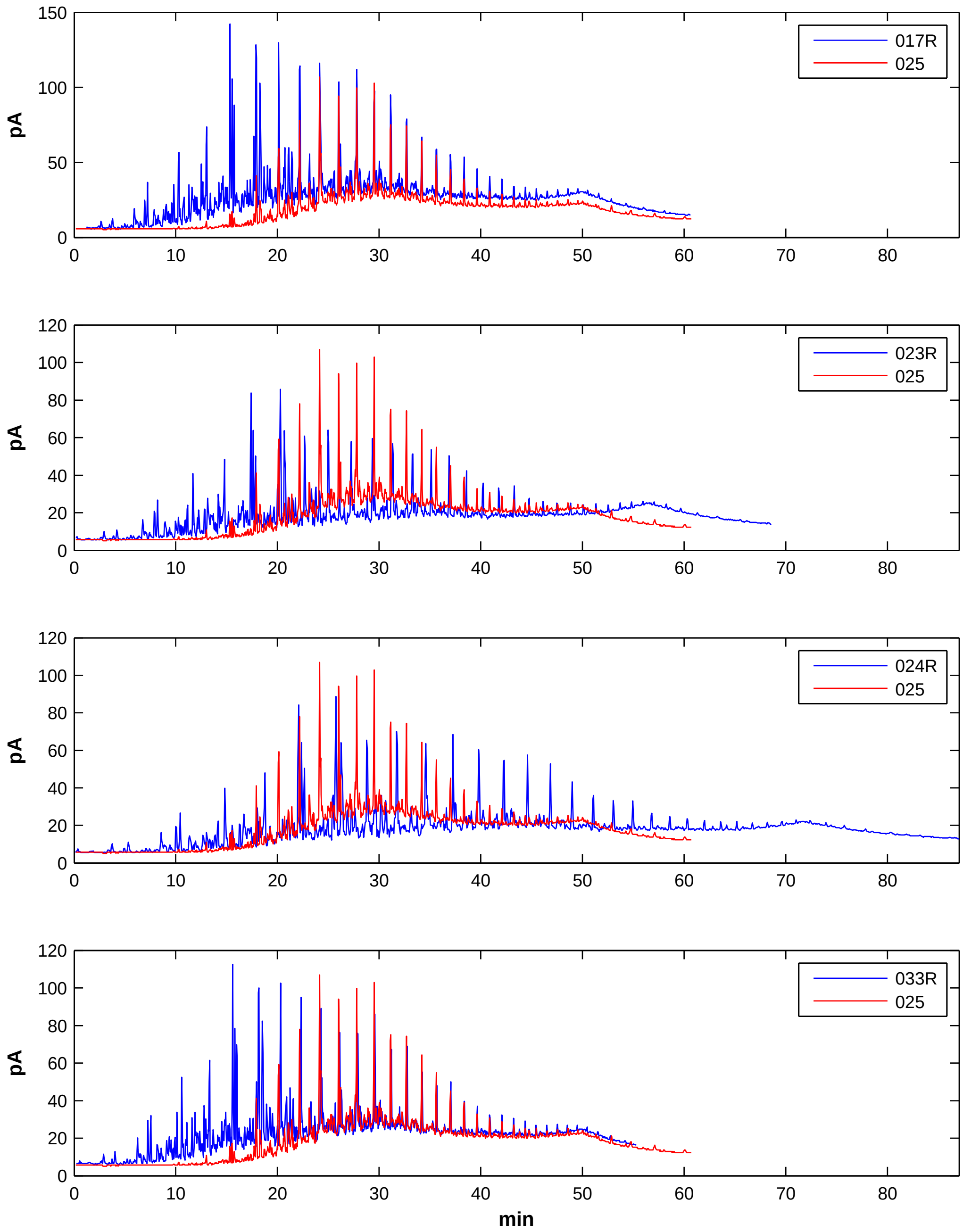

Figure B.12: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0025) and the reference samples.

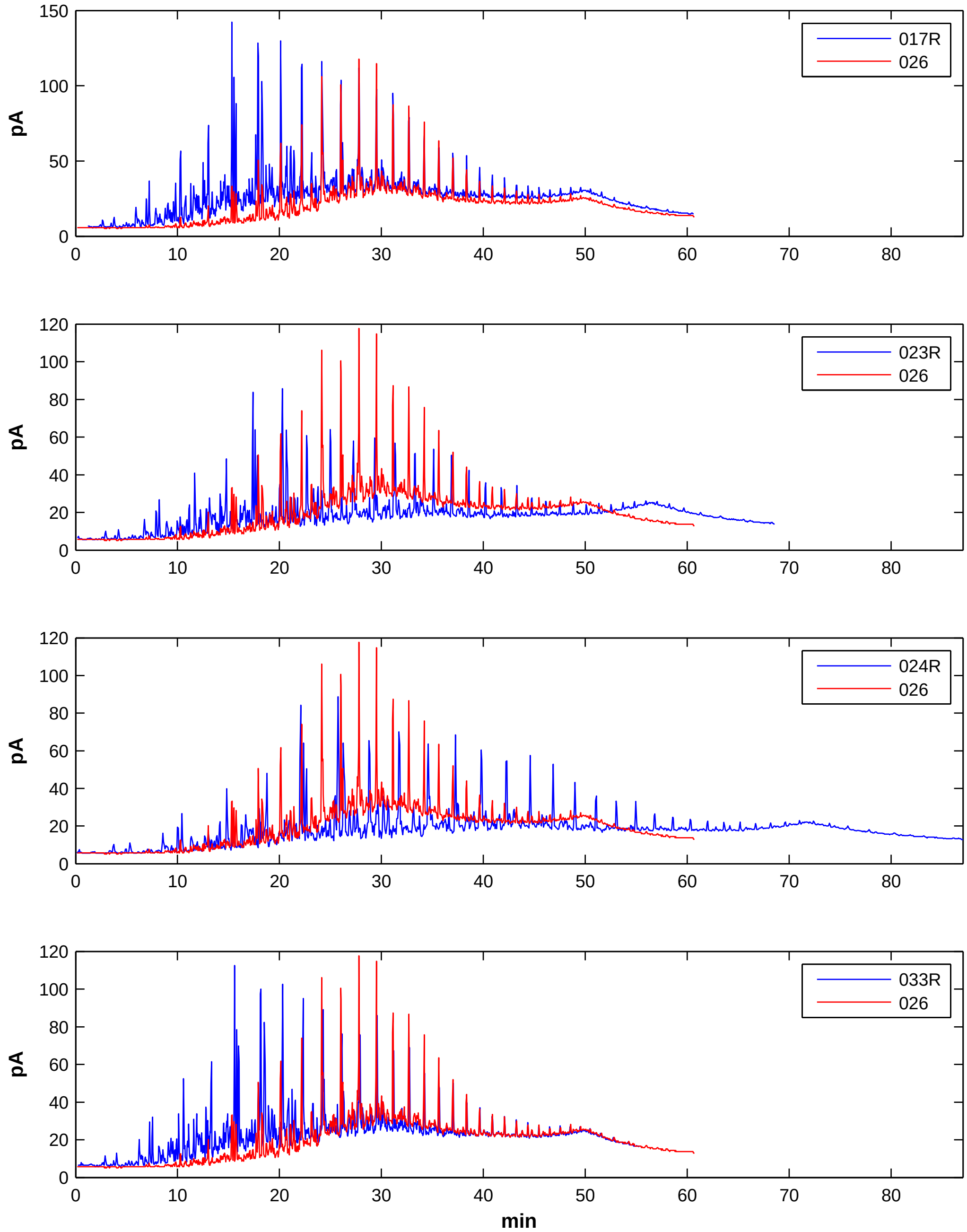

Figure B.13: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0026) and the reference samples.

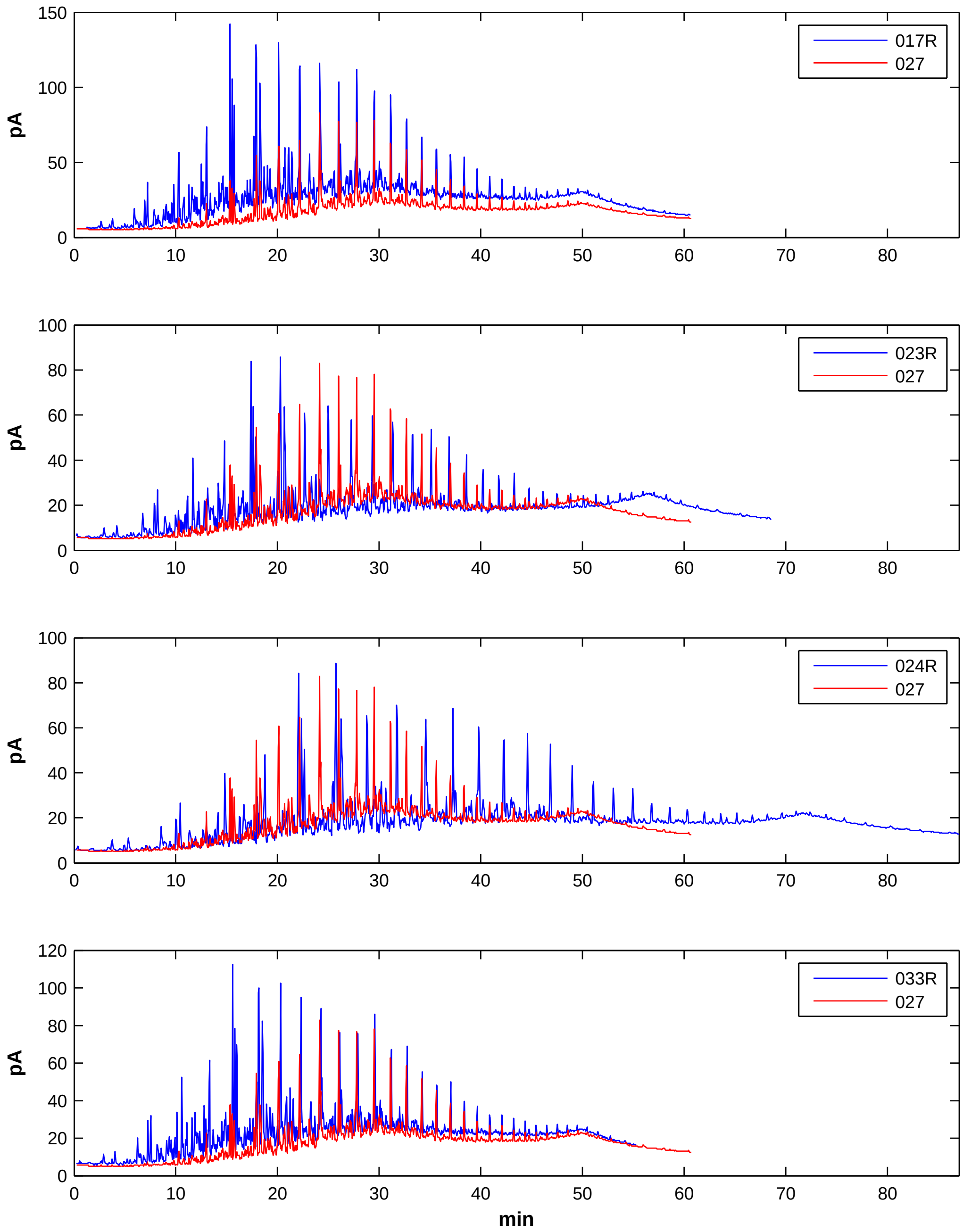

Figure B.14: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0027) and the reference samples.

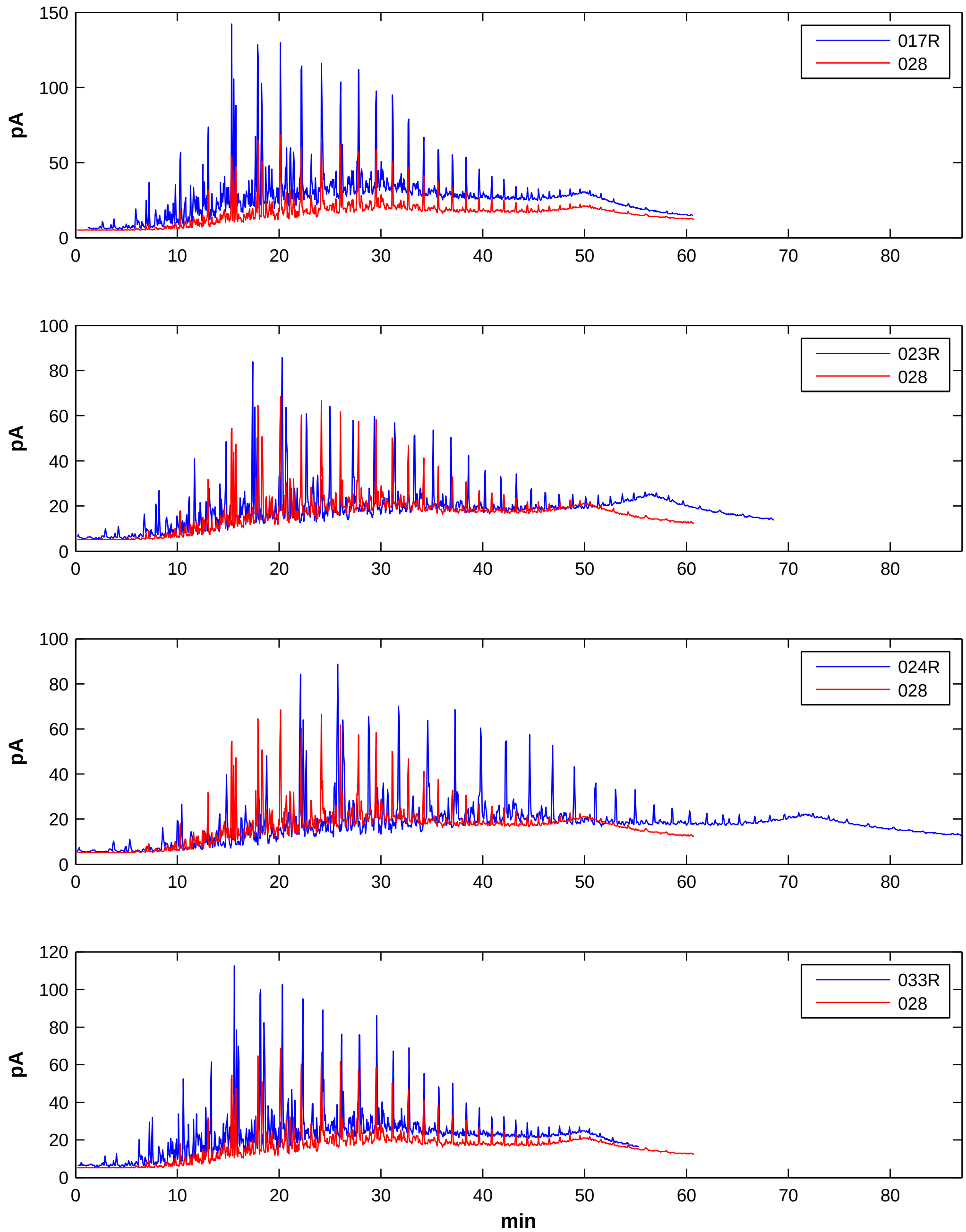

Figure B.15: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0028) and the reference samples.

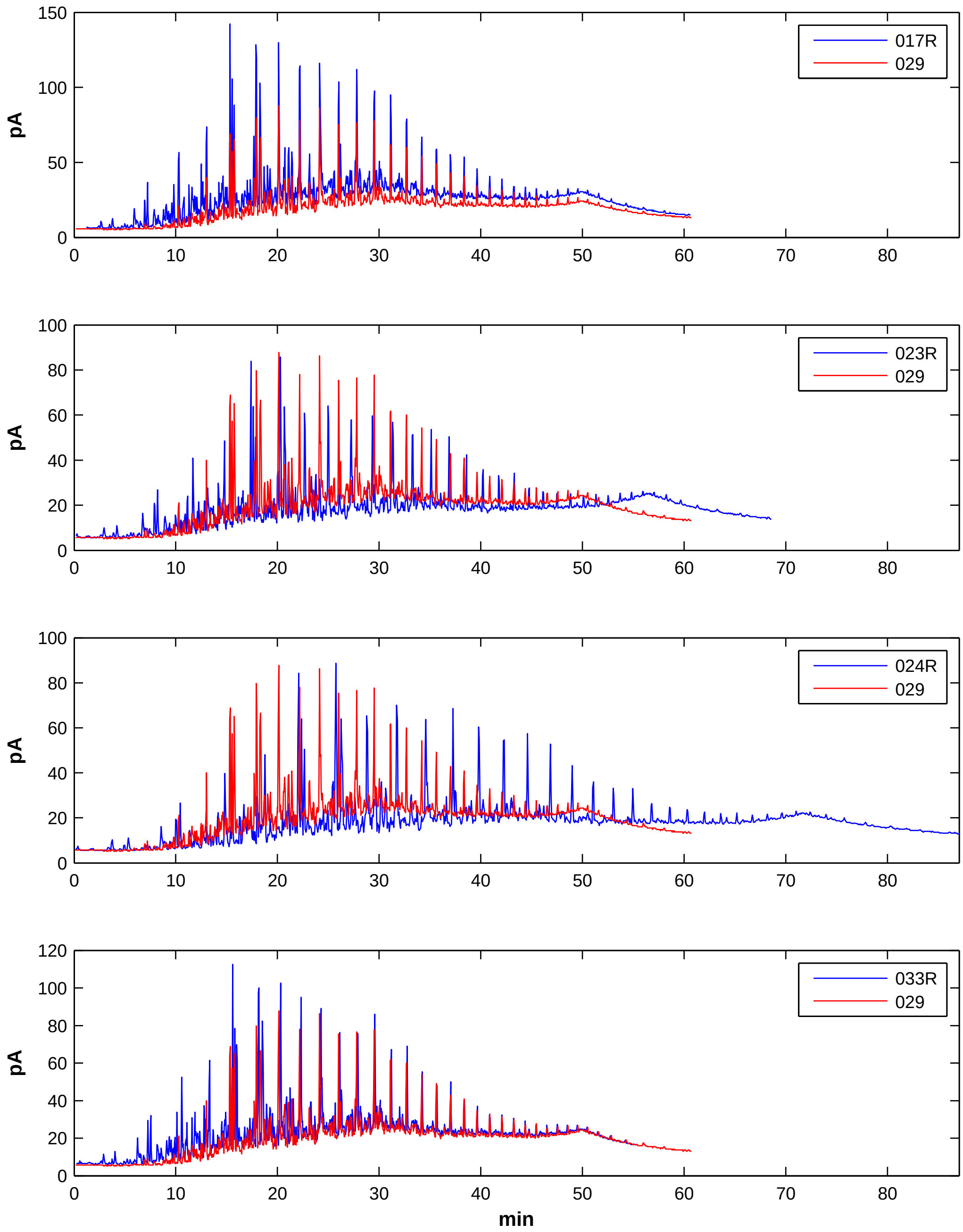

Figure B.16: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0029) and the reference samples.

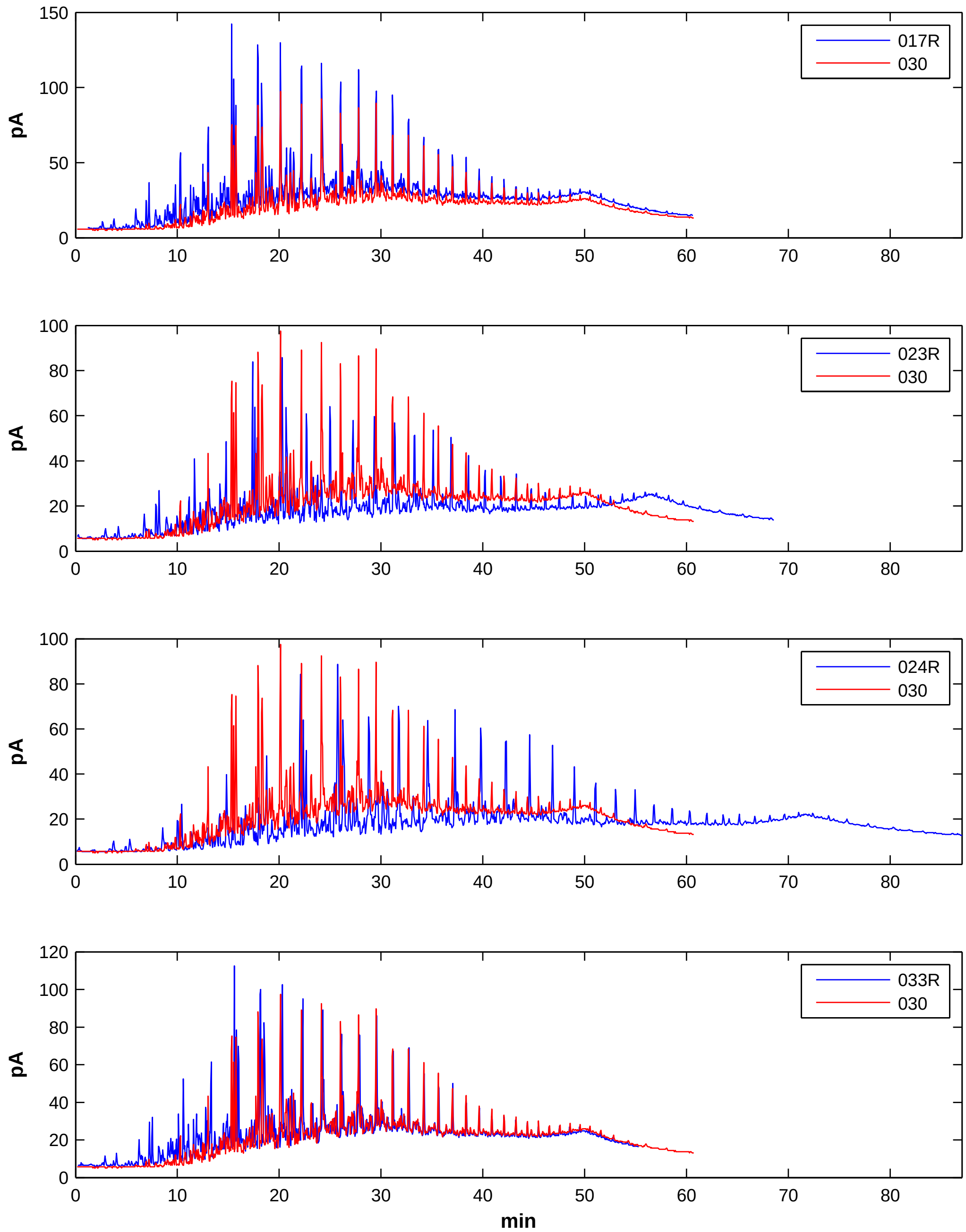

Figure B.17: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0030) and the reference samples.

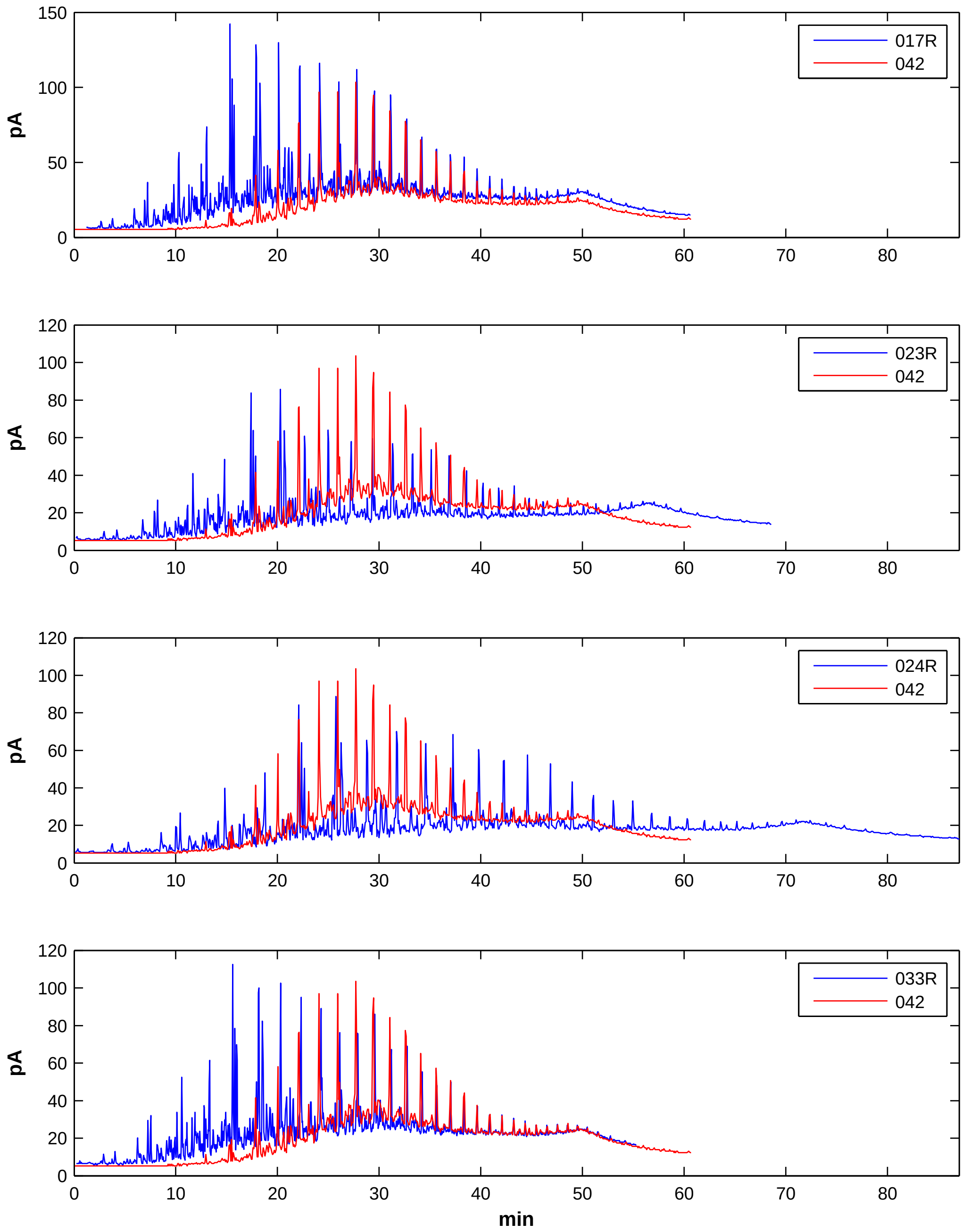

Figure B.18: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0042) and the reference samples.

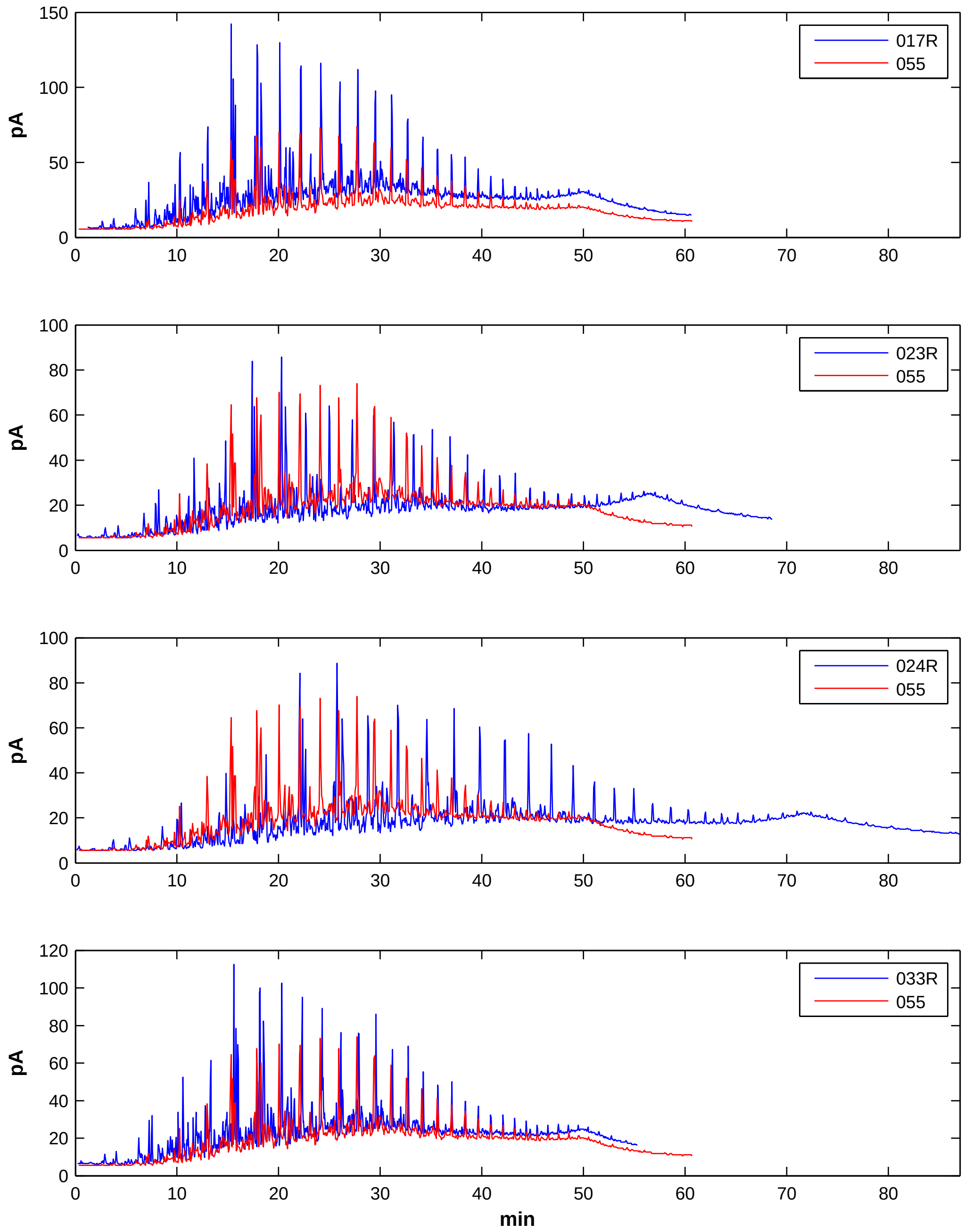

Figure B.19: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0055) and the reference samples.

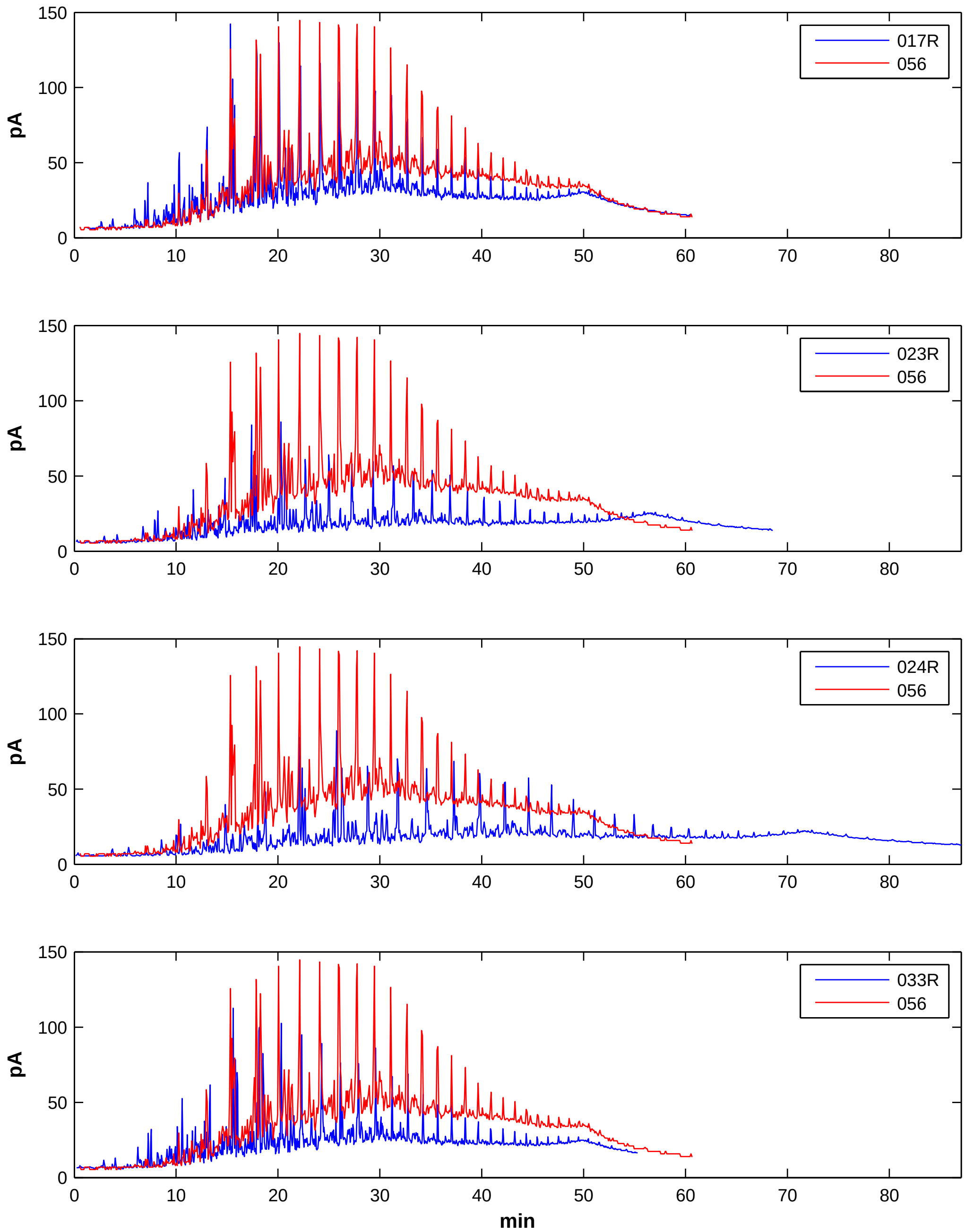

Figure B.20: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0056) and the reference samples.

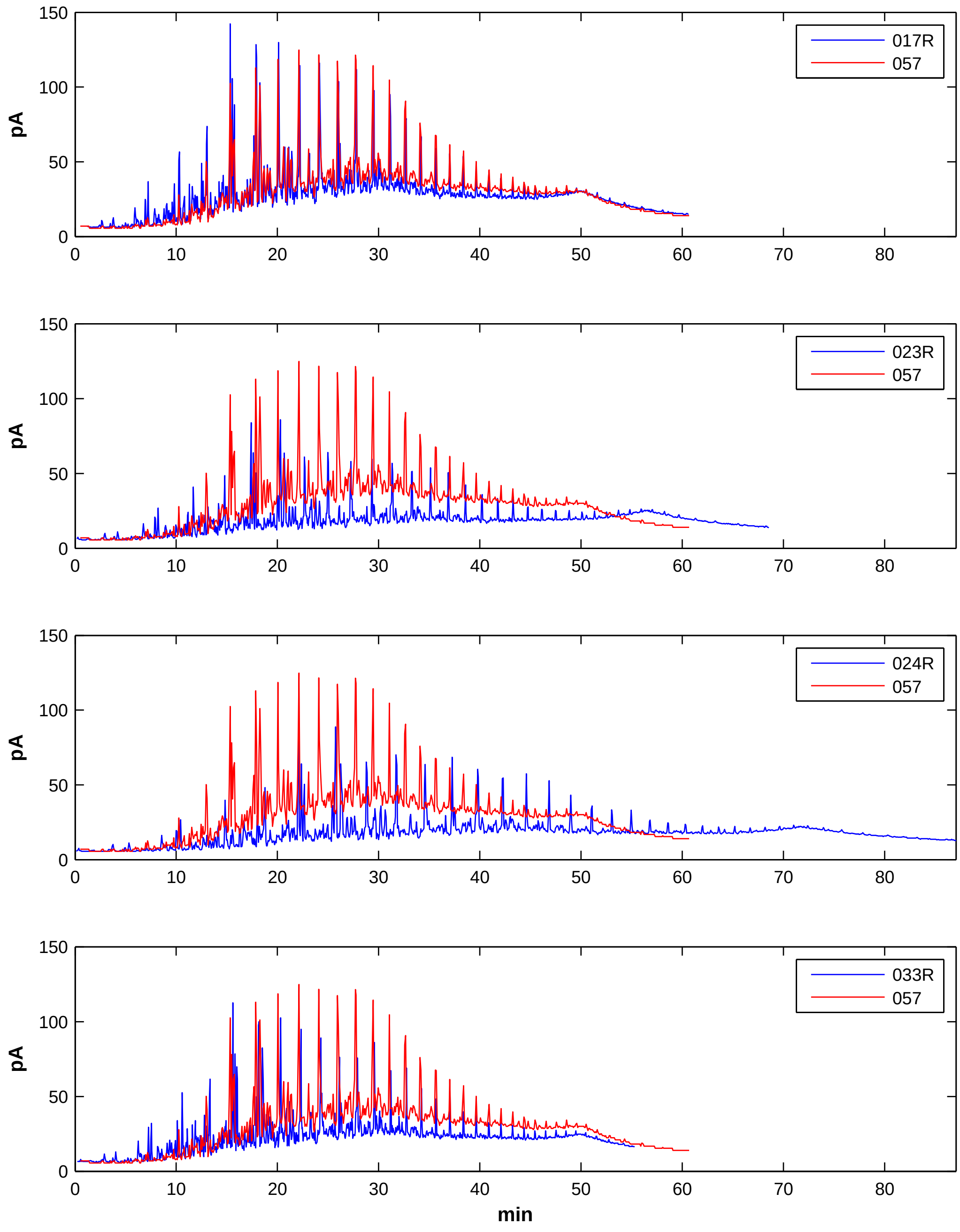

Figure B.21: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0057) and the reference samples.

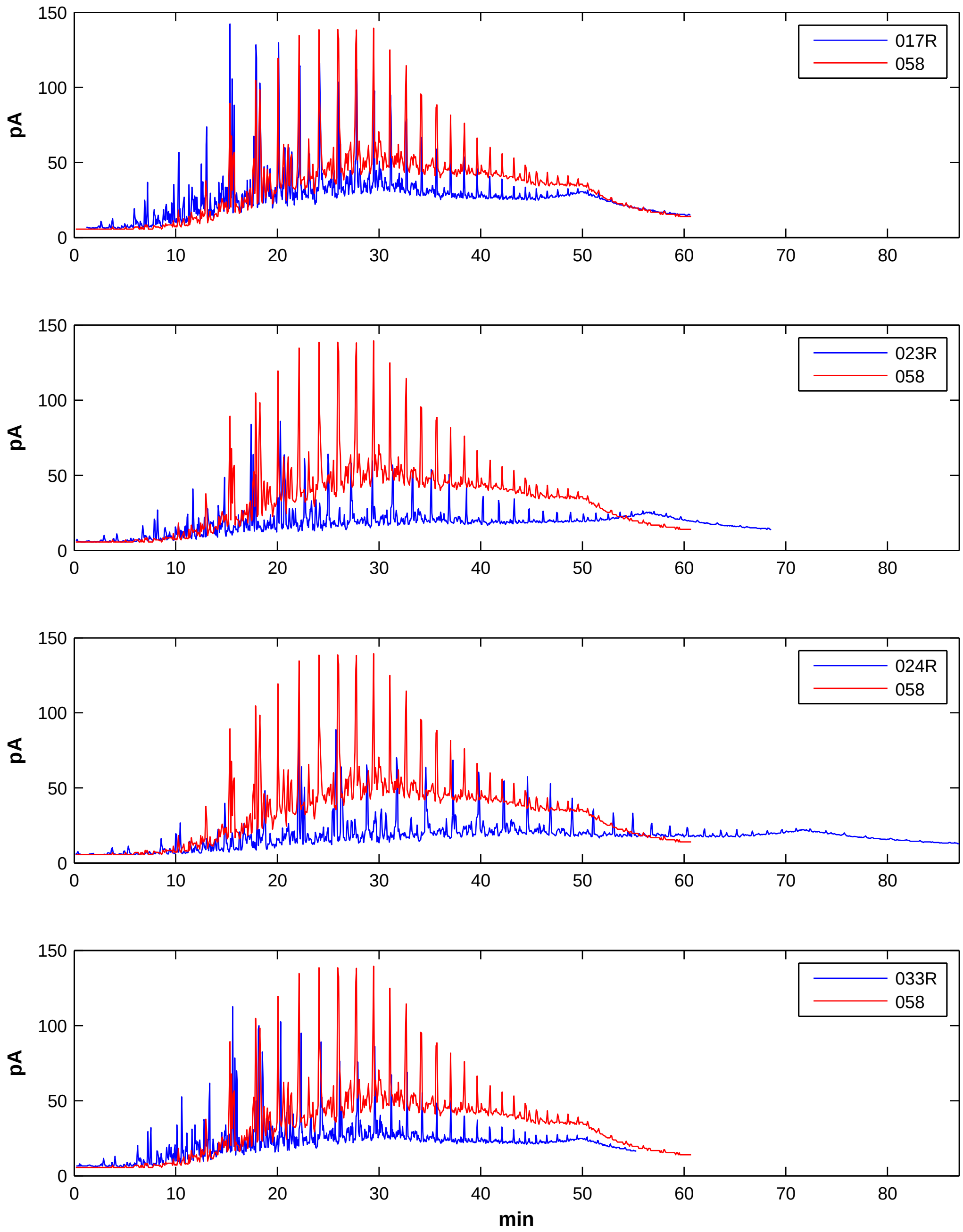

Figure B.22: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0058) and the reference samples.

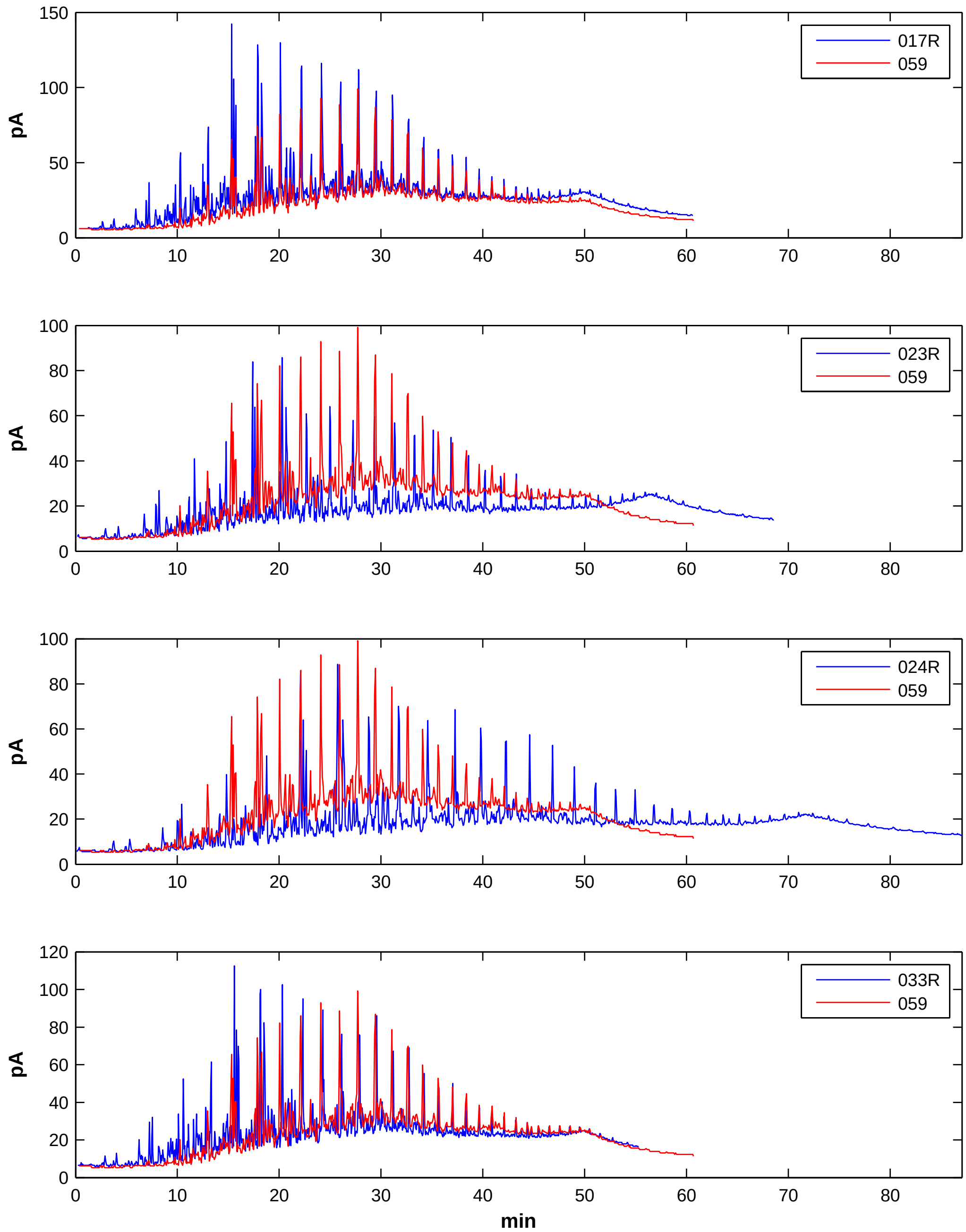

Figure B.23: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0059) and the reference samples.

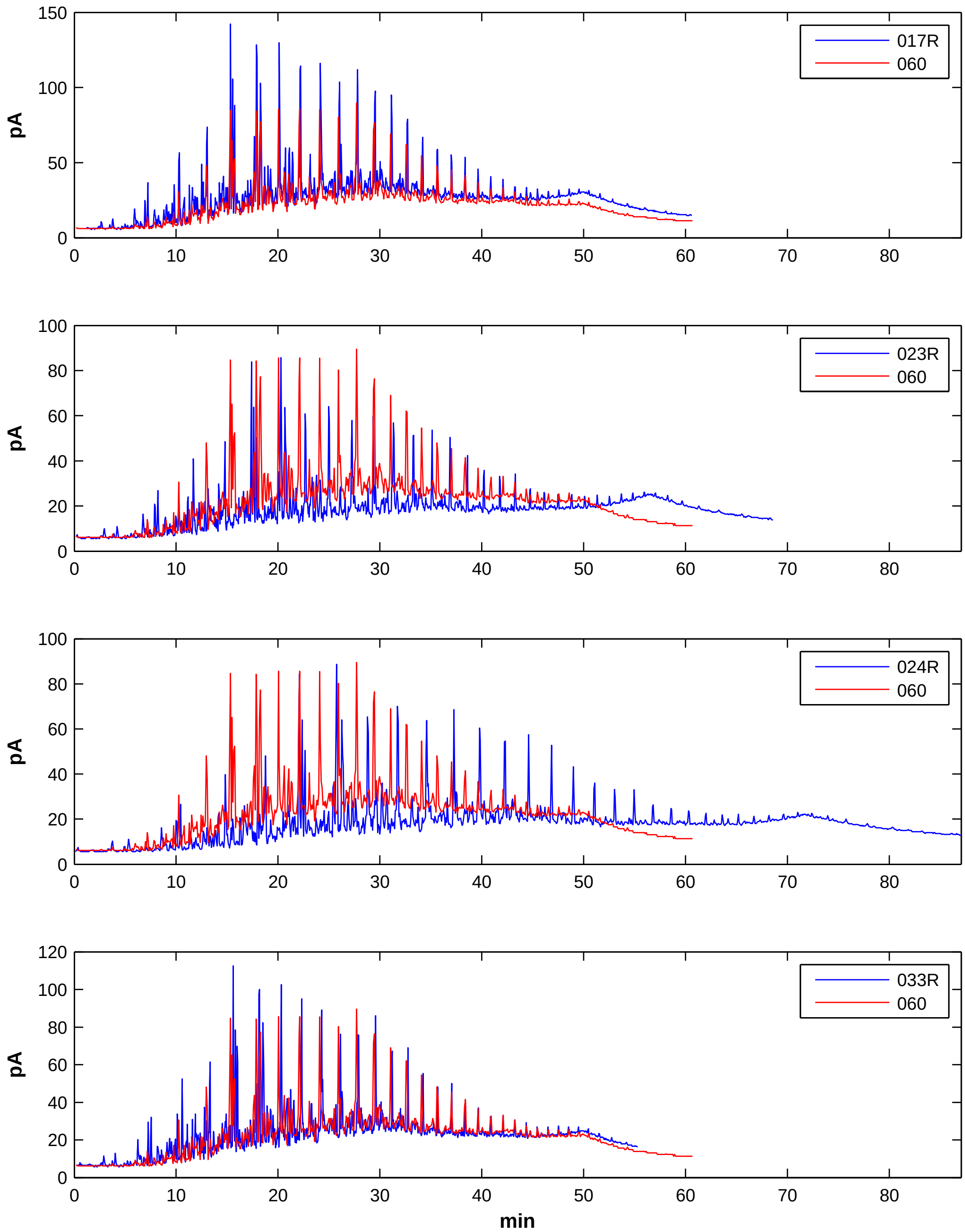

Figure B.24: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0060) and the reference samples.

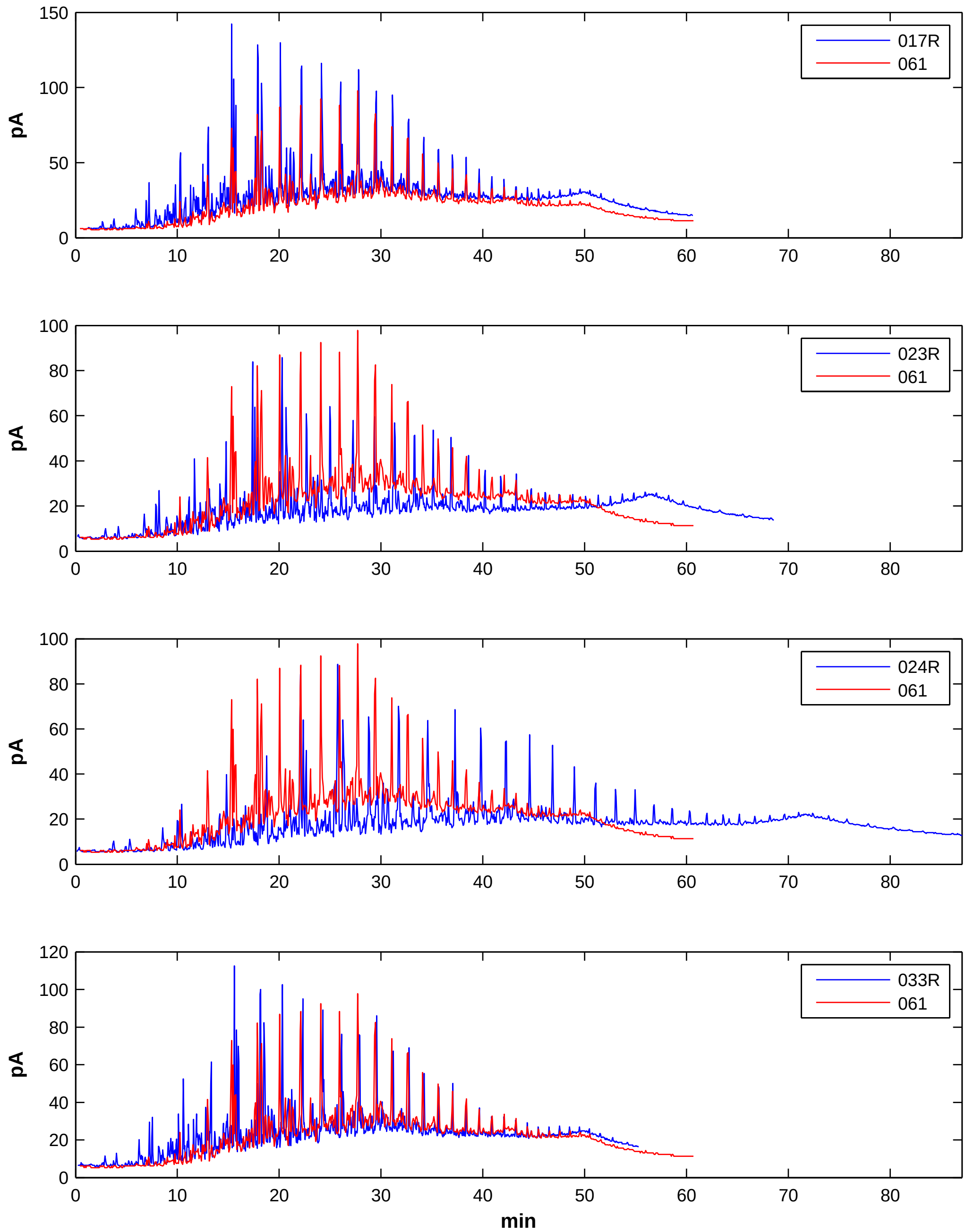

Figure B.25: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0061) and the reference samples.

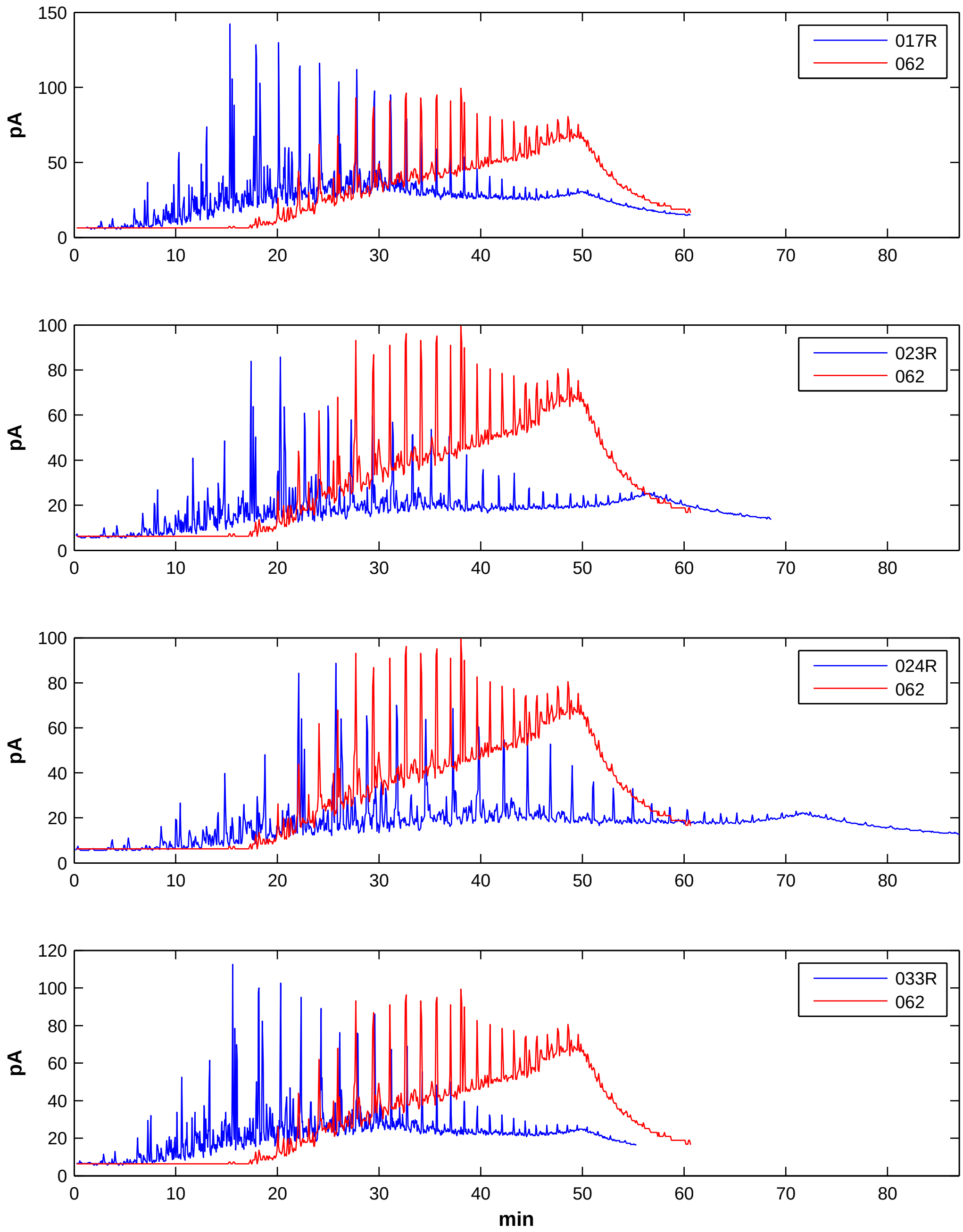

Figure B.26: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0062) and the reference samples.

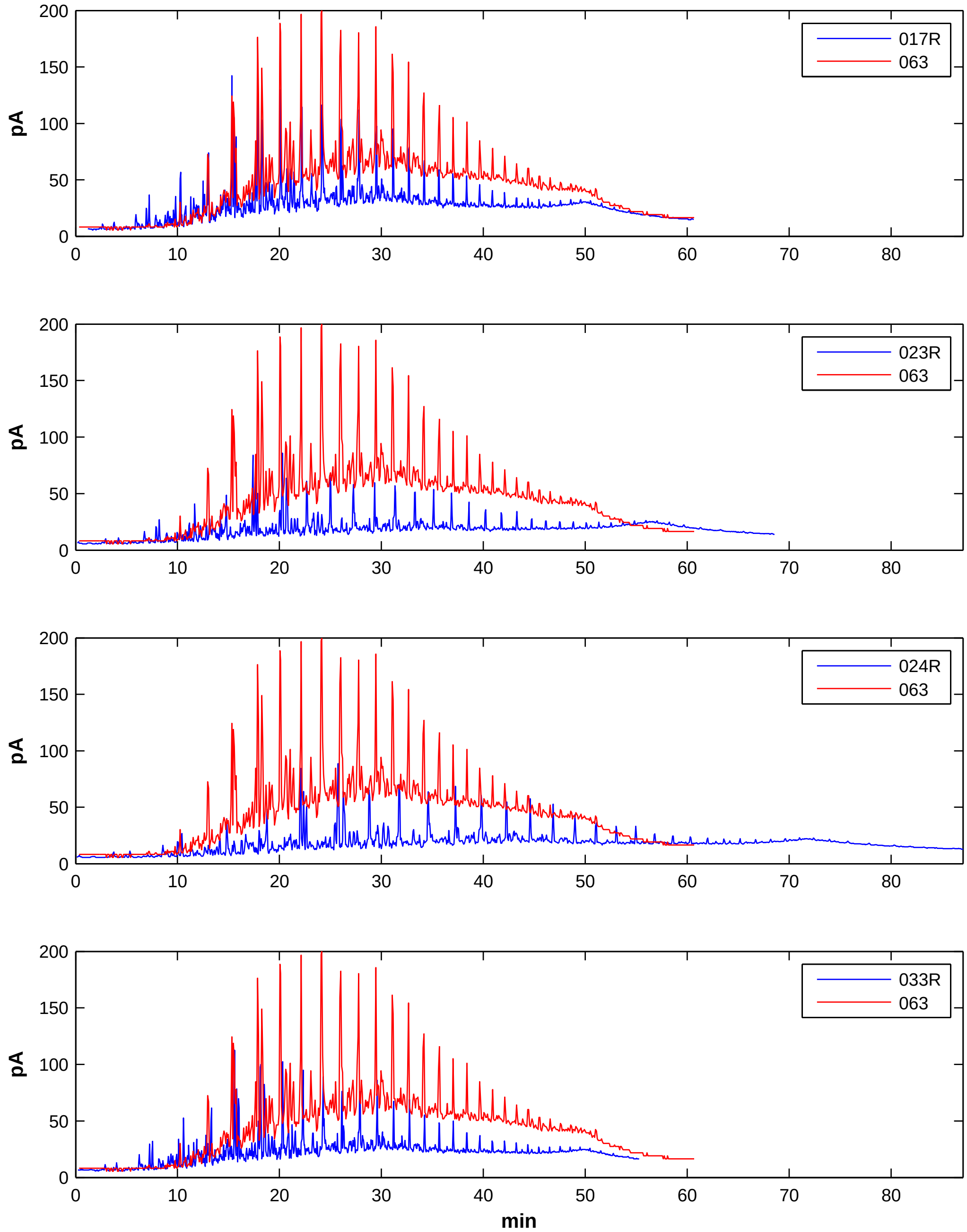

Figure B.27: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0063) and the reference samples.

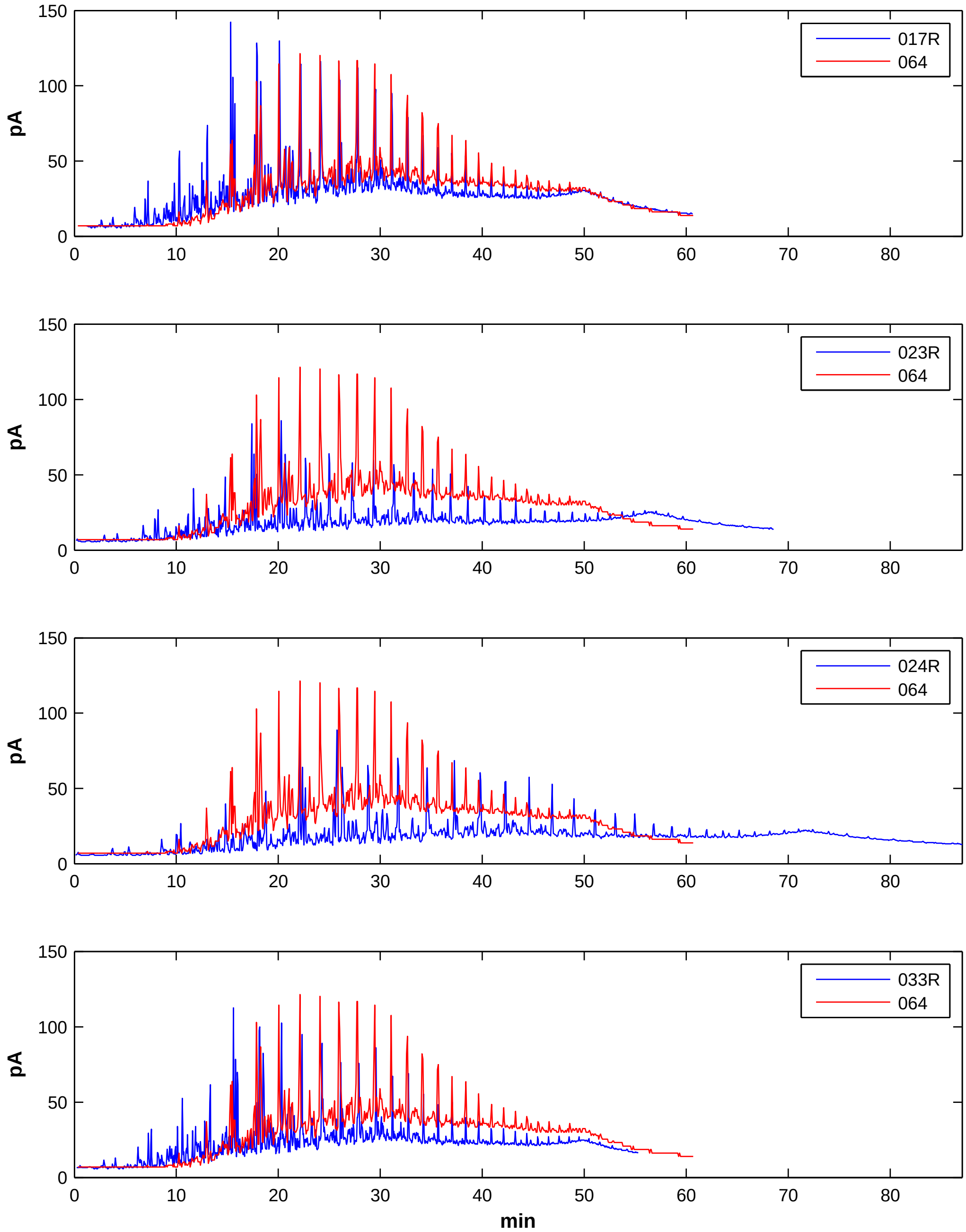

Figure B.28: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0064) and the reference samples.

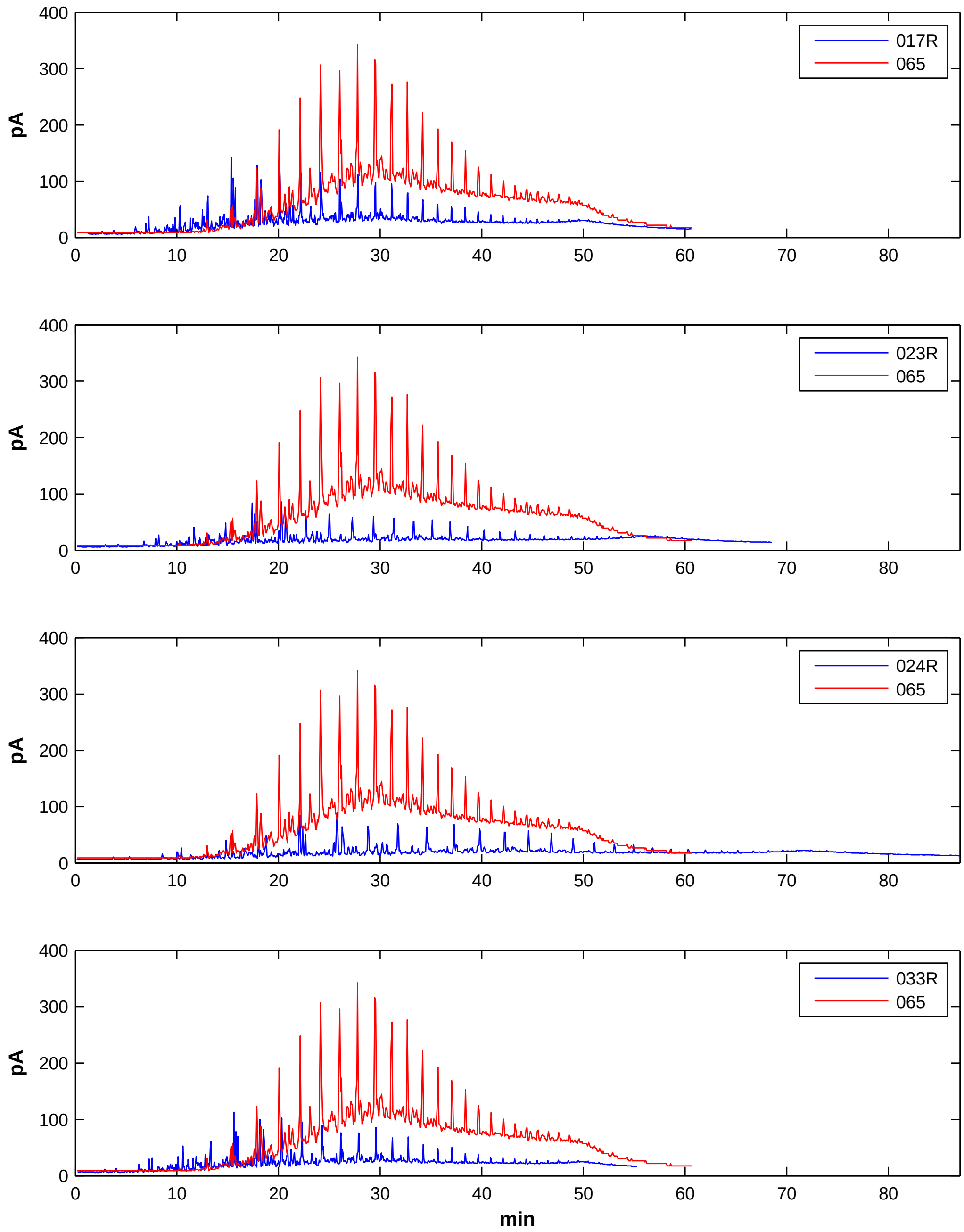

Figure B.29: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0065) and the reference samples.

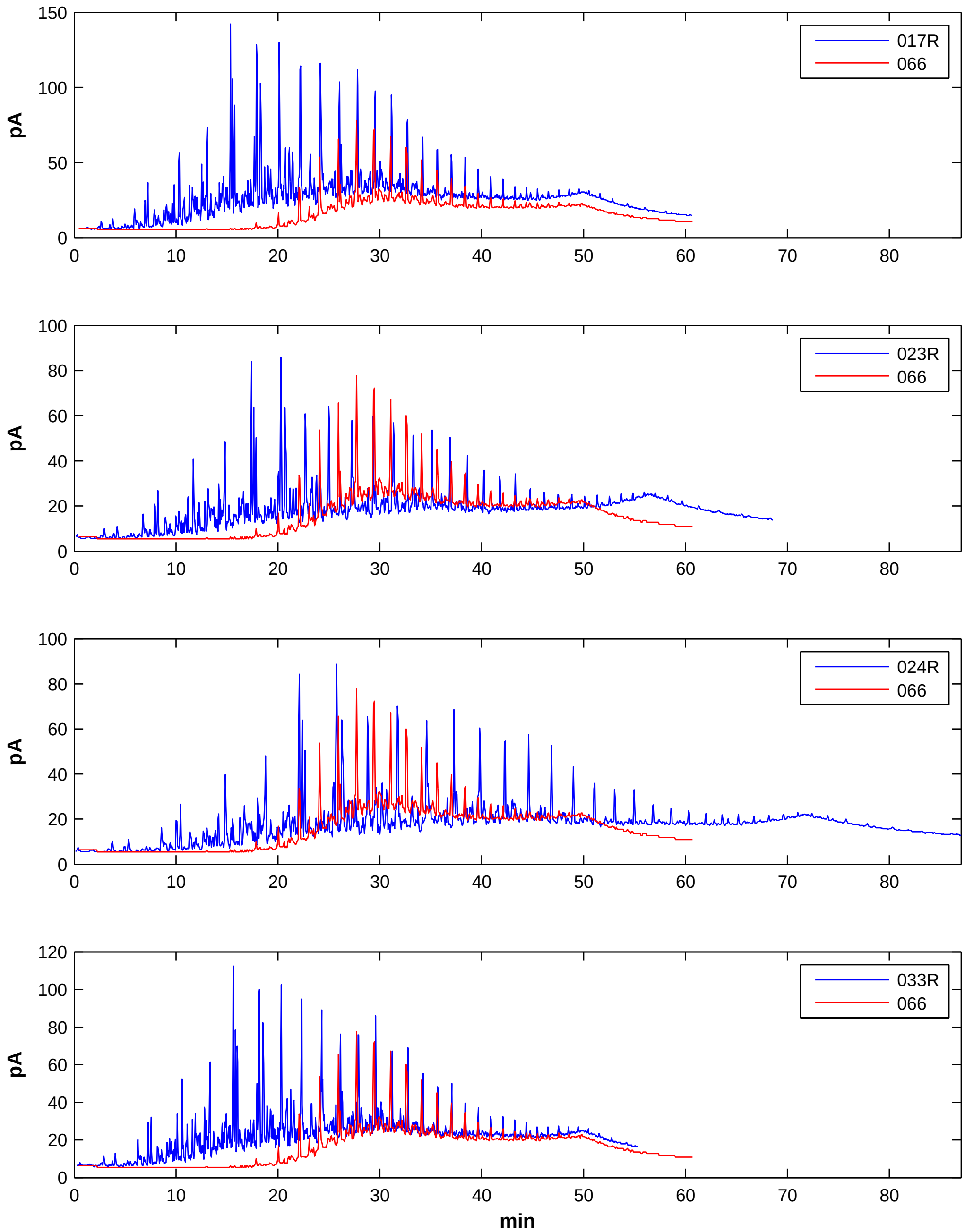

Figure B.30: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0066) and the reference samples.

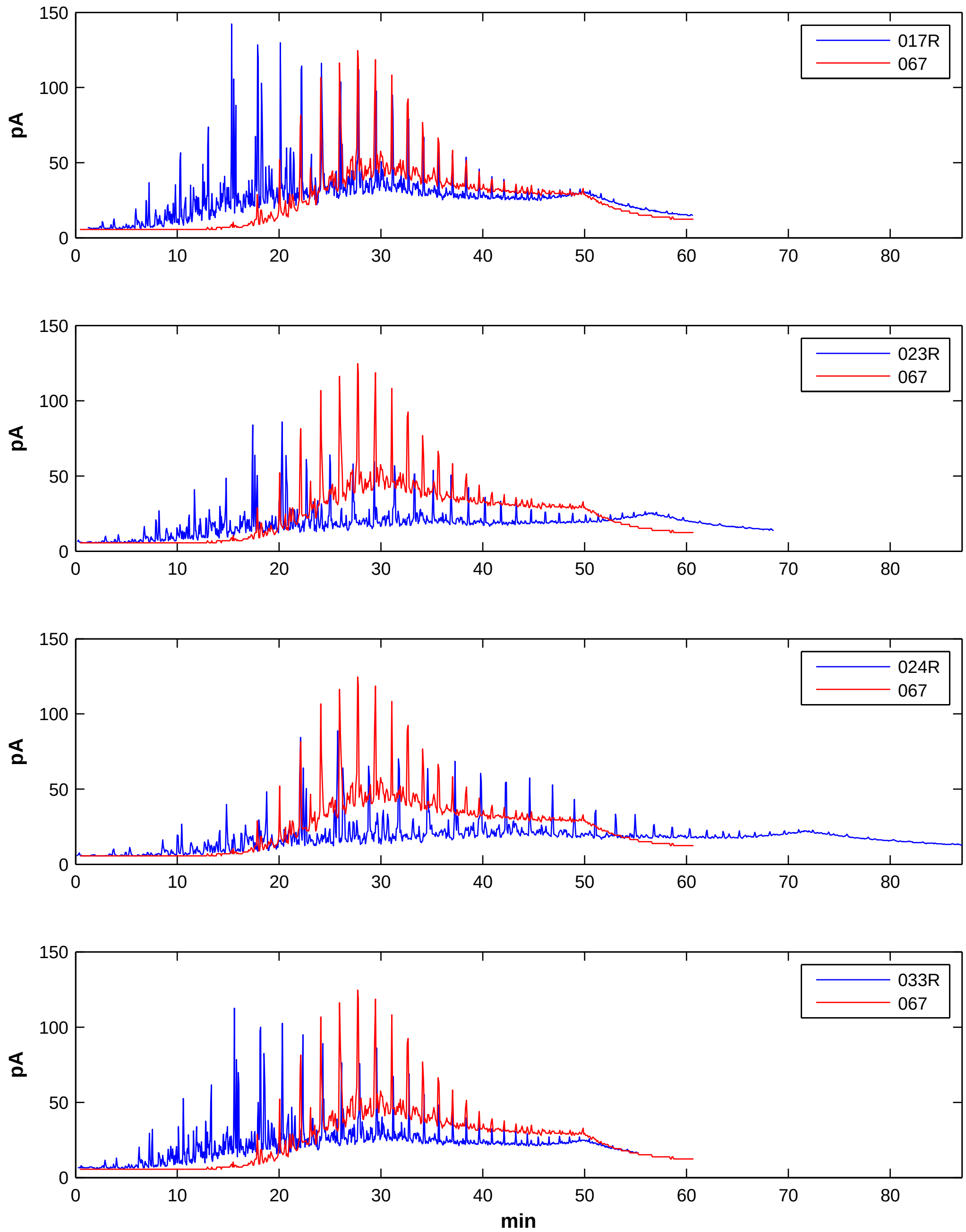

Figure B.31: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0067) and the reference samples.

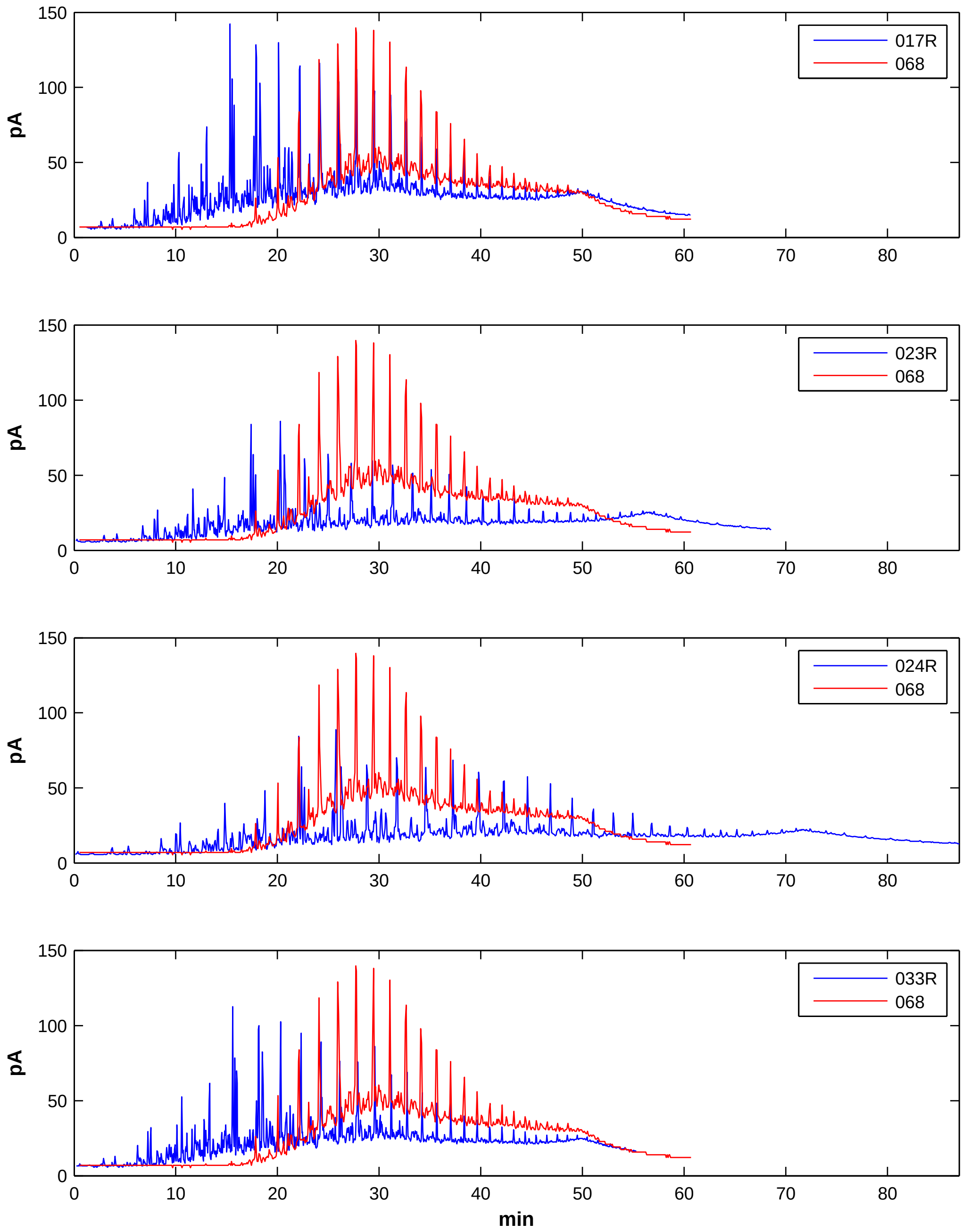

Figure B.32: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0068) and the reference samples.

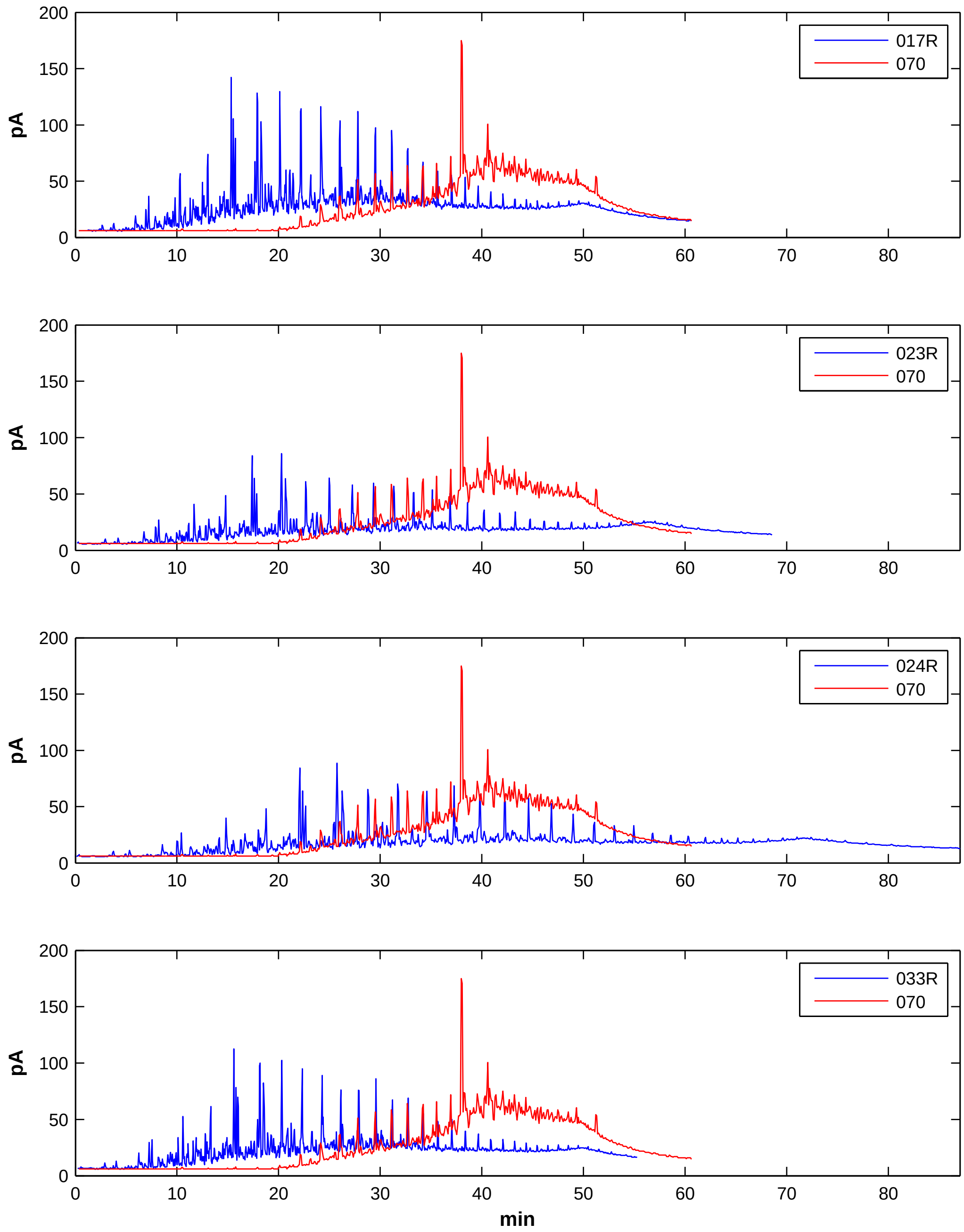

Figure B.33: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0070) and the reference samples.

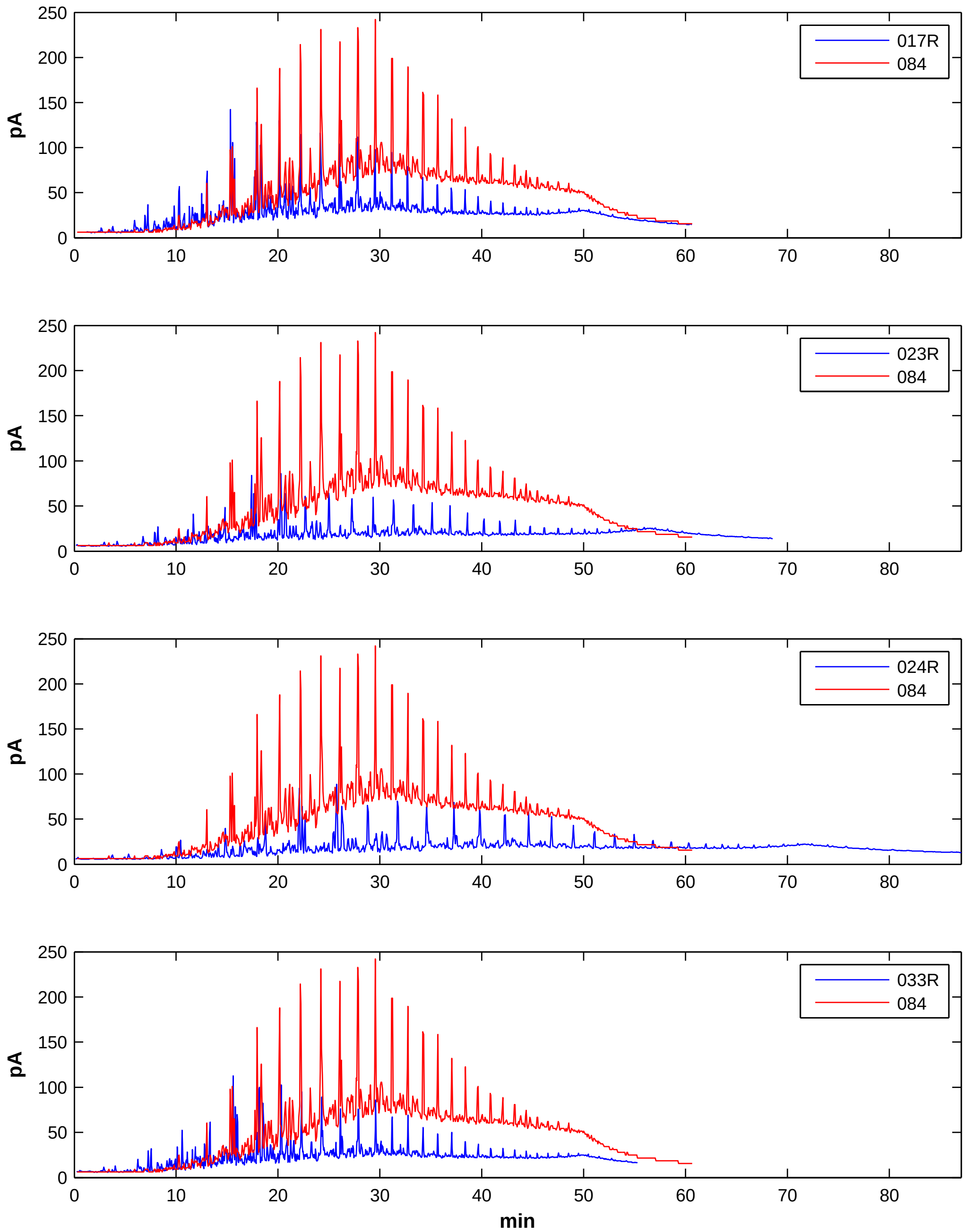

Figure B.34: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0084) and the reference samples.

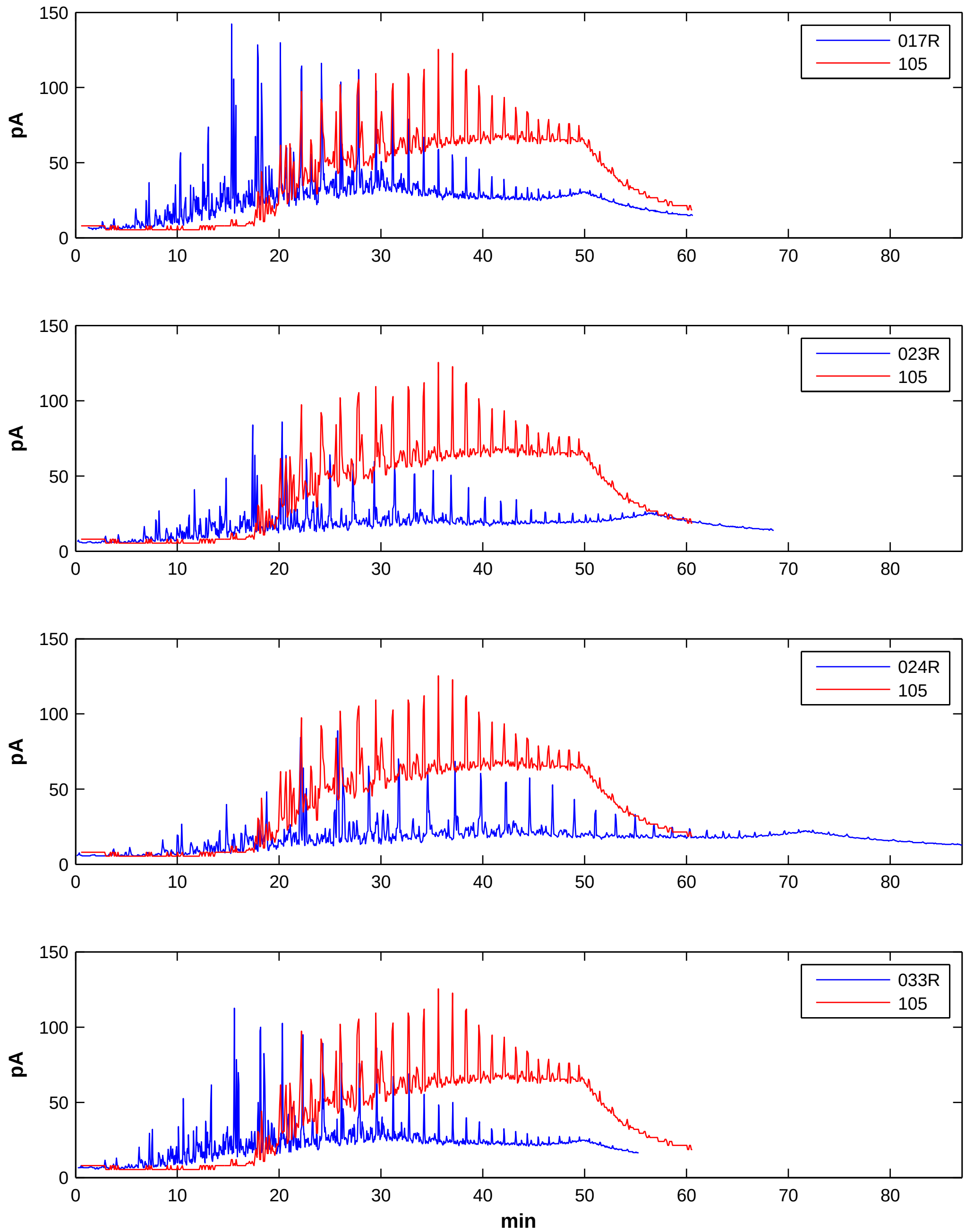

Figure B.35: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0105) and the reference samples.

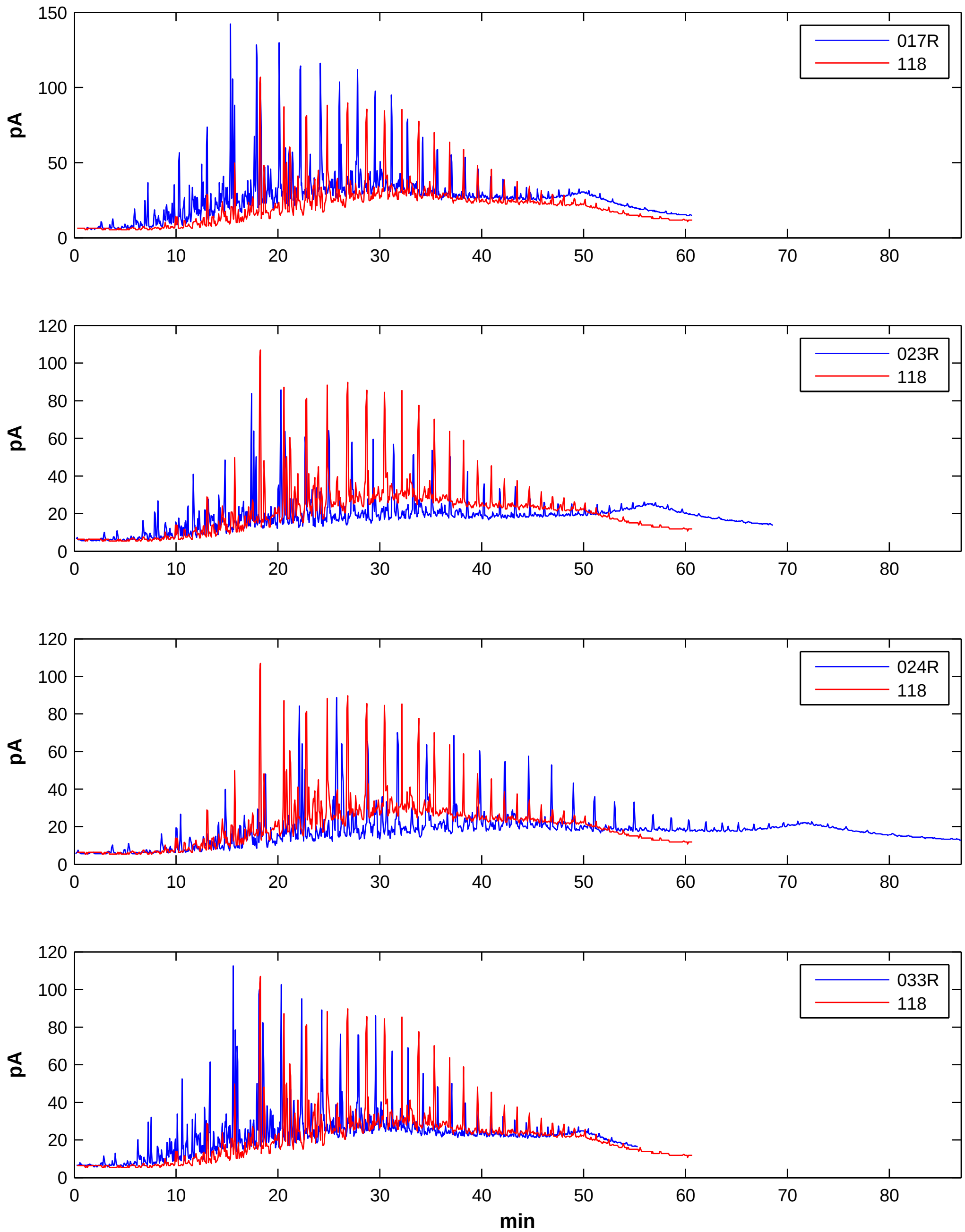

Figure B.36: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0118) and the reference samples.

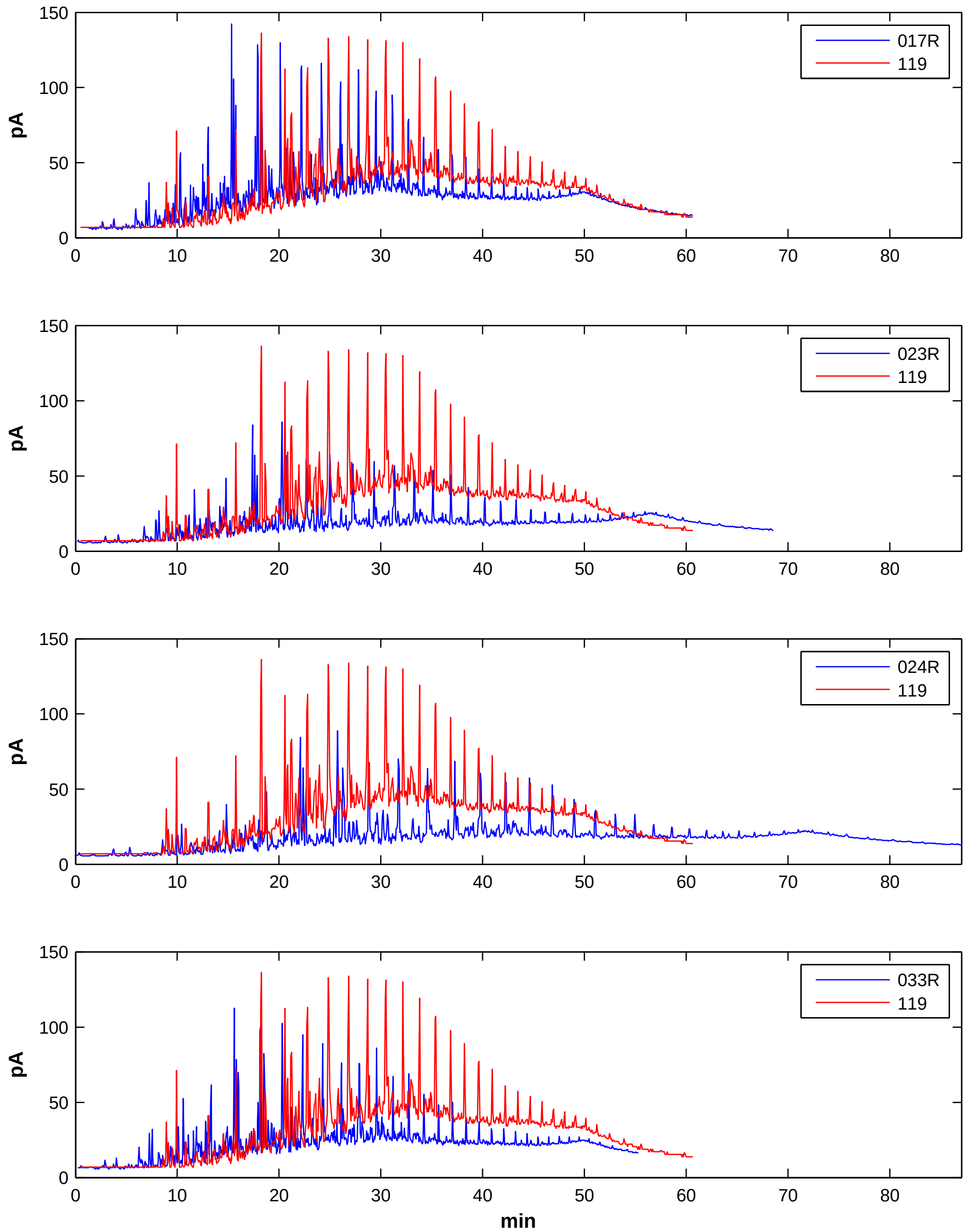

Figure B.37: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0119) and the reference samples.

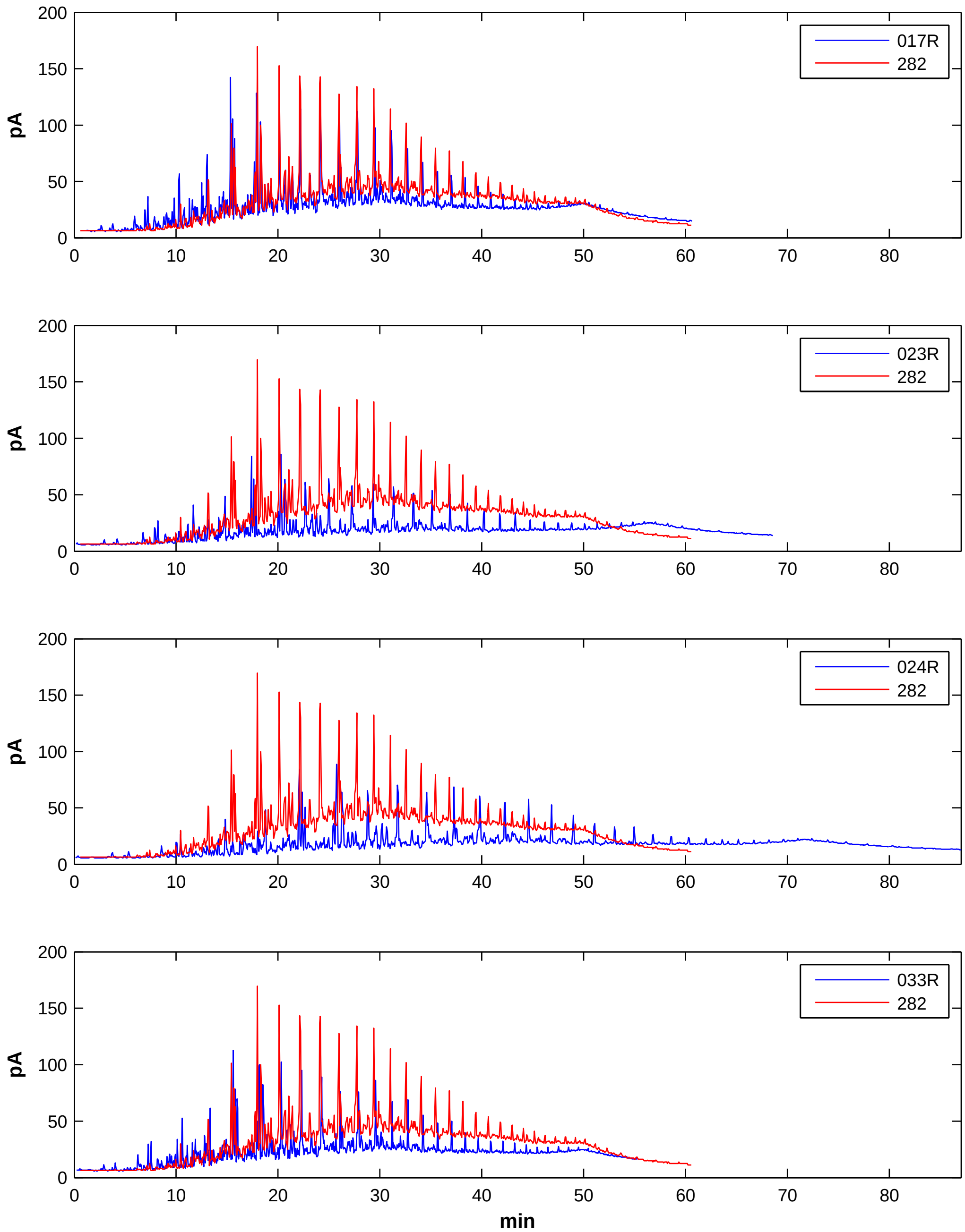

Figure B.38: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0282) and the reference samples.

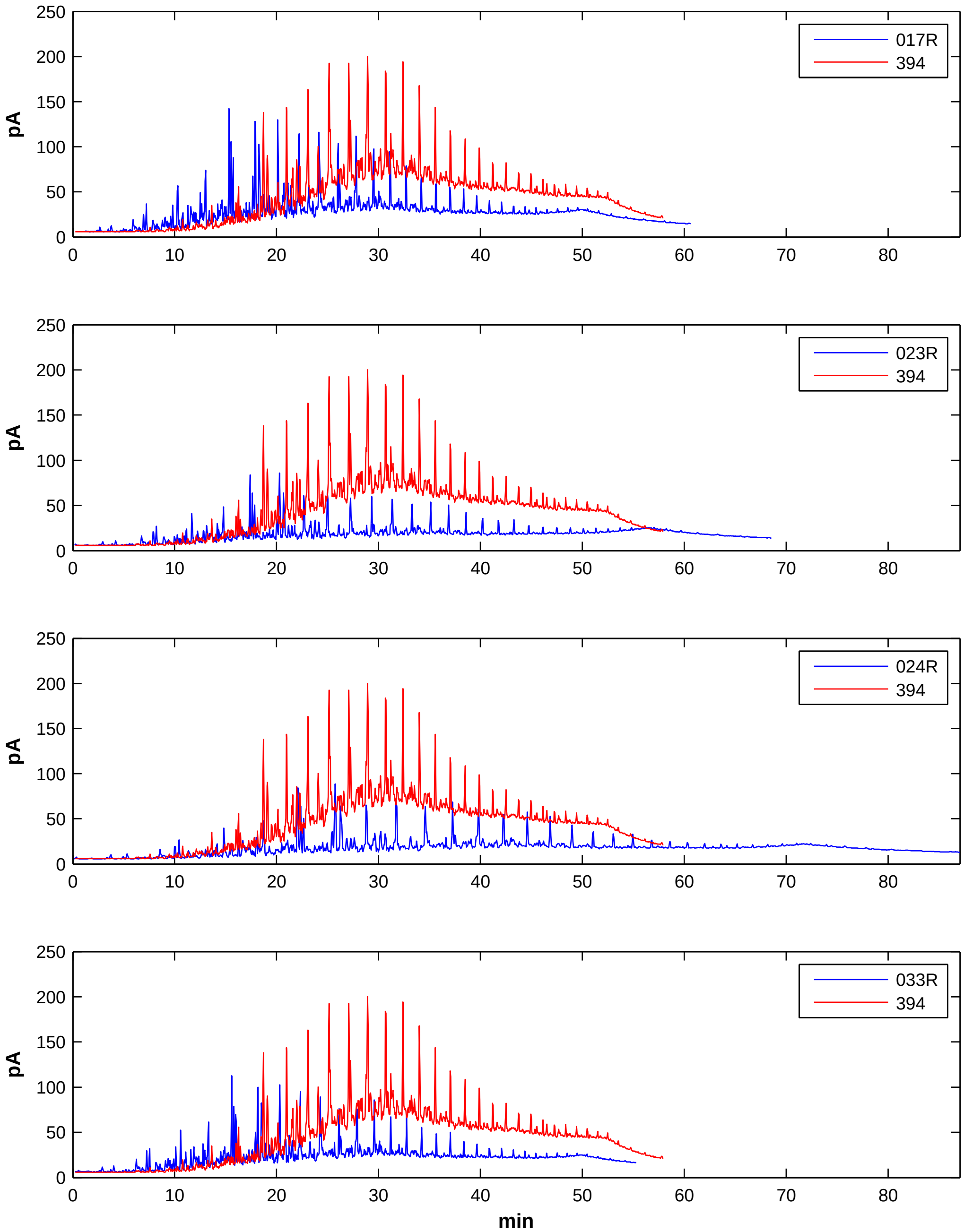

Figure B.39: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0394) and the reference samples.

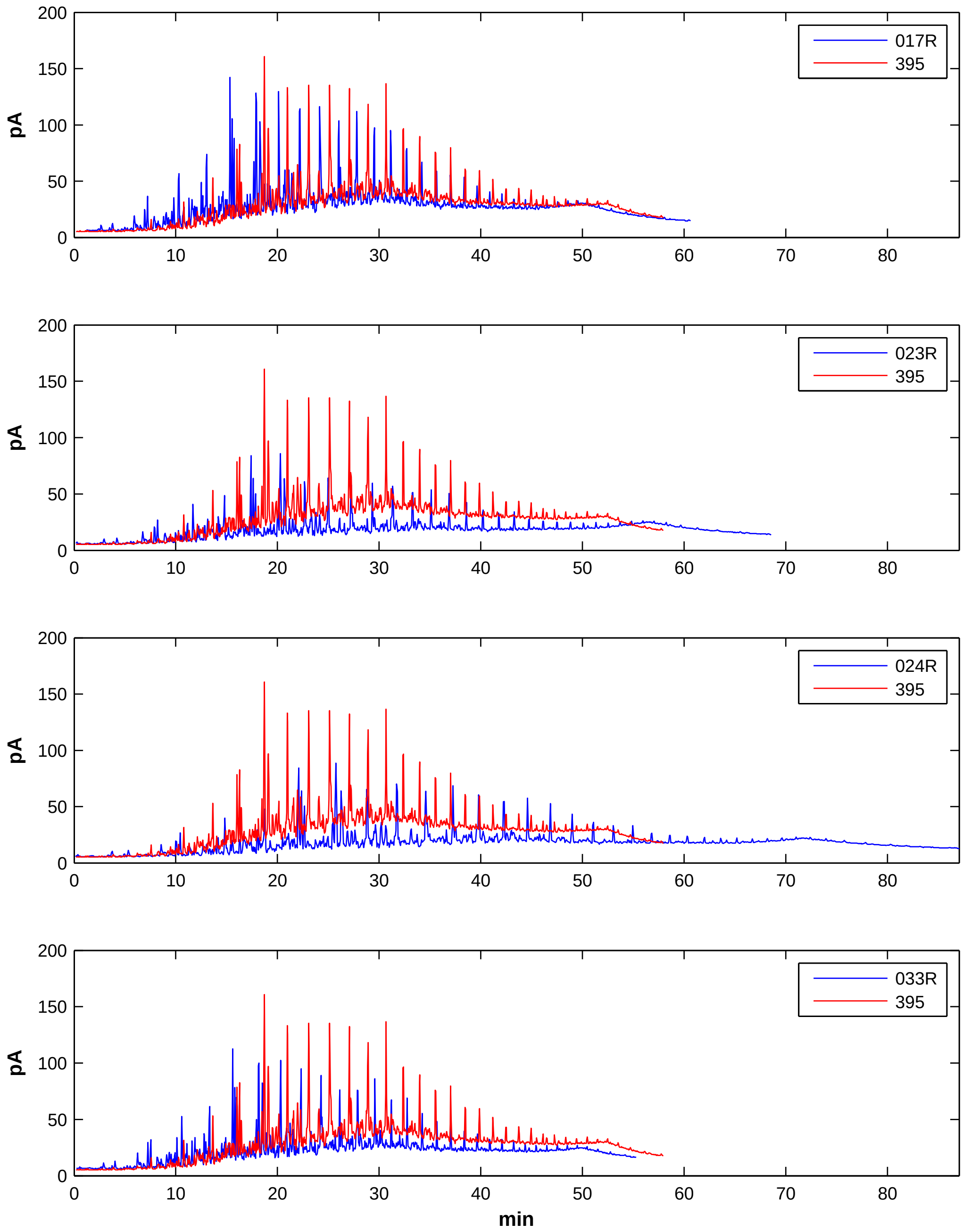

Figure B.40: Overlaying of the GC/FID chromatograms of the oil spill sample (SINTEF ID: 2007-0395) and the reference samples.

C AVAILABLE DATA ON DIAGNOSTIC RATIO OF "FULL CITY" AND "SERVER" CASE

The available data of diagnostic ratio in the form of *.xls files is presented in the following Fig. C.1 and C.2 for "Full City" and "Server" case respectively.

Table C.1: Diagnostic Ratio of "Full City" Case.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
C28tricycllics	1.00	0.97	0.98	0.91	0.99	1.00	0.93	0.98	0.92	1.00	0.97	0.85	0.84	1.09	1.00	0.97	nd	nd
C29 tricyclics	1.08	0.98	1.01	1.48	1.95	3.92	1.92	2.98	1.17	0.97	0.92	0.96	0.93	1.10	1.05	1.04	nd	nd
C28+C29tricyclics	2.07	2.00	1.97	1.73	1.67	1.45	1.66	1.49	1.89	1.92	1.99	2.01	1.93	2.21	2.22	1.99	nd	nd
27Ts	0.34	0.52	0.50	0.62	0.45	0.34	0.51	0.52	0.49	0.61	0.56	0.79	0.71	0.54	0.19	0.48	0.50	0.89
28ab	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.11
25nor30ab	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.08
29ab	0.82	0.73	0.73	0.70	0.75	0.80	0.70	0.72	0.74	0.73	0.74	0.96	0.68	0.58	0.74	0.74	0.67	0.87
29Ts	0.12	0.15	0.14	0.16	0.14	0.13	0.14	0.15	0.15	0.16	0.16	0.18	0.16	0.17	0.10	0.15	0.12	0.21
30d	0.04	0.05	0.05	0.05	0.04	0.03	0.04	0.05	0.05	0.05	0.05	0.03	0.06	0.09	0.04	0.05	0.05	0.06
30O	0.12	0.03	0.04	0.00	0.07	0.13	0.04	0.04	0.04	0.00	0.00	0.12	0.00	0.09	0.00	0.05	0.00	0.00
30G	0.00	0.10	0.09	0.10	0.09	0.08	0.09	0.09	0.09	0.00	0.11	0.10	0.12	0.08	0.07	0.09	0.00	0.00
29ba	0.08	0.06	0.07	0.05	0.07	0.08	0.06	0.06	0.06	0.07	0.06	0.08	0.06	0.08	0.09	0.06	0.06	0.33
29aaS	0.85	0.98	0.96	0.98	0.93	0.85	0.92	0.98	0.93	0.97	0.98	0.87	1.01	0.74	0.93	0.92	0.83	1.15
29bb	1.35	1.36	1.35	1.33	1.33	1.38	1.29	1.33	1.28	1.41	1.39	1.61	1.57	1.04	1.12	1.34	1.40	1.70
27bbSTER	0.53	0.51	0.53	0.51	0.52	0.52	0.52	0.49	0.51	0.50	0.48	0.38	0.39	0.57	0.65	0.51	0.54	0.47
28bbSTER	0.36	0.37	0.37	0.37	0.37	0.34	0.37	0.38	0.37	0.39	0.36	0.32	0.33	0.40	0.38	0.37	0.36	0.40
29bbSTER	0.64	0.65	0.62	0.65	0.63	0.68	0.63	0.65	0.65	0.63	0.69	0.93	0.89	0.54	0.50	0.64	0.63	0.65
TA21	0.80	0.45	0.49	0.40	0.53	0.86	0.49	0.46	0.46	0.41	0.39	0.53	0.22	1.71	1.28	0.48	2.71	0.55
TA26	0.52	0.48	0.45	0.45	0.46	0.49	0.46	0.44	0.44	0.44	0.43	0.41	0.25	0.58	0.61	0.44	0.44	0.33
TA27	0.93	0.87	0.87	0.85	0.86	0.90	0.85	0.86	0.89	0.88	0.85	0.73	0.44	0.89	1.02	0.87	0.80	1.02
2-MP/1-MP	2.20	1.89	2.00	1.42	1.99	1.98	1.90	1.90	1.91	1.65	1.55	1.97	1.63	1.85	1.94	1.95	1.91	1.22
4-MD/1-MD	2.75	2.54	2.53	2.16	2.67	2.65	2.53	2.51	2.52	2.30	2.07	3.14	2.93	2.93	2.25	2.48	3.00	2.66
C2-dbt/C2-phe	0.36	0.40	0.38	0.51	0.38	0.38	0.37	0.38	0.38	0.45	0.42	0.49	0.33	0.27	0.26	0.43	0.35	0.20
C3-dbt/C3-phe	0.50	0.60	0.56	0.63	0.51	0.54	0.55	0.57	0.54	0.61	0.59	0.64	0.40	0.34	0.40	0.56	0.43	0.25
C3-dbt/C3-chr	2.19	2.39	2.42	2.03	2.26	2.55	2.20	2.38	2.15	2.00	2.13	2.38	1.39	0.84	2.20	2.38	21.62	1.25
Retene/C4-phe	0.07	0.02	0.02	0.04	0.02	0.04	0.02	0.02	0.02	0.04	0.05	0.03	0.05	0.04	0.02	0.02	0.04	0.40
B(a)F/4-Mpy	0.32	0.46	0.39	0.92	0.35	0.35	0.40	0.41	0.40	0.64	0.64	0.39	0.82	0.52	0.27	0.42	0.57	1.97
B(b+c)F/4-Mpy	0.18	0.24	0.19	0.43	0.19	0.18	0.20	0.19	0.19	0.32	0.31	0.22	0.39	0.28	0.15	0.20	0.31	0.94
2Mpy/4-Mpy	1.13	1.02	1.05	0.79	1.08	1.13	1.05	1.03	1.04	0.90	0.77	1.18	0.90	0.96	0.91	1.05	1.08	1.11
1Mpy/4-Mpy	0.94	0.91	0.90	0.86	0.91	0.89	0.91	0.88	0.89	0.89	0.84	0.96	0.89	0.89	0.85	0.89	0.89	0.69

*Note: number 1...18 represents the sample of 2009-0485, 2009-0472, 2009-0486, 2009-0489, 2009-0491, 2009-0493, 2009-0499, 2009-0500, 2009-0501, 2009-0602, 2009-0604, 2009-0606, 2009-0609, 2009-0614, 2009-0616, 2009-0622, 2004-0355, 2009-0626

Table C.2: Diagnostic Ratio of "Server" Case.

SINTEF ID	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34
2007-0017	0.22	0.16	0.39	0.52	0.15	0.07	0.90	0.16	0.05	0.09	0.14	0.07	0.87	0.98	0.75	0.31	0.51	4.86	0.44	1.03	2.14	2.43	0.63	0.80	2.95	0.04	0.46	0.28	0.95	0.93	1.62	0.46	1.05	0.90
2007-0017a	0.20	0.15	0.34	0.51	0.12	0.06	0.92	0.15	0.04	0.08	0.13	0.07	0.87	0.93	0.71	0.32	0.52	4.99	0.43	1.06	2.14	2.42	0.63	0.77	2.80	0.05	0.46	0.27	0.97	0.91	1.64	0.43	0.99	0.89
2007-0022	0.18	0.15	0.33	0.71	0.11	0.07	0.86	0.18	0.05	0.36	0.11	0.08	0.95	0.92	0.70	0.33	0.51	3.17	0.21	1.07	2.09	2.30	0.59	0.73	2.12	0.04	0.47	0.30	0.91	0.91	1.57	0.48	1.10	1.04
2007-0022a	0.18	0.15	0.32	0.74	0.12	0.06	0.87	0.18	0.05	0.36	0.11	0.08	0.90	0.99	0.68	0.33	0.53	2.96	0.21	1.00	2.08	2.30	0.59	0.73	2.05	0.04	0.46	0.29	0.91	0.91	1.60	0.51	1.06	0.99
2007-0023	0.19	0.16	0.35	0.53	0.12	0.06	0.90	0.16	0.04	0.12	0.13	0.08	0.88	0.94	0.70	0.34	0.50	4.04	0.51	1.03	2.17	2.45	0.67	0.83	2.62	0.04	0.46	0.26	0.97	0.92	1.83	0.38	0.98	0.96
2007-0023a	0.21	0.16	0.37	0.51	0.12	0.06	0.94	0.16	0.04	0.12	0.12	0.07	0.89	0.90	0.74	0.32	0.50	3.96	0.48	1.05	2.17	2.46	0.67	0.83	3.36	0.04	0.45	0.28	0.96	0.92	nd	0.39	1.00	0.98
2007-0024	0.24	0.17	0.41	0.54	0.14	0.06	0.87	0.15	0.04	0.09	0.13	0.08	0.86	0.98	0.76	0.32	0.48	4.64	0.44	1.02	2.15	2.41	0.61	0.77	2.62	0.04	0.46	0.28	0.95	0.97	nd	0.40	0.92	0.93
2007-0033	0.23	0.16	0.40	0.51	0.14	0.06	0.93	0.16	0.04	0.10	0.13	0.07	0.92	0.92	0.74	0.31	0.51	4.60	0.43	1.03	2.15	2.44	0.63	0.78	2.84	0.05	0.46	0.28	0.98	0.93	1.72	0.41	0.96	0.94
2007-0018	0.26	0.19	0.45	0.54	0.16	0.07	0.86	0.14	0.05	0.04	0.15	0.07	0.98	1.18	0.83	0.31	0.44	5.63	0.53	1.08	2.10	2.35	0.52	0.64	2.29	0.05	0.46	0.28	0.97	0.94	1.26	0.24	0.75	0.48
2007-0019	0.22	0.17	0.40	0.54	0.12	0.06	0.87	0.15	0.04	0.08	0.13	0.07	0.91	0.97	0.74	0.32	0.49	4.82	0.43	1.07	2.14	2.42	0.61	0.76	2.98	0.04	0.46	0.27	0.97	0.92	nd	nd	nd	nd
2007-0021	0.23	0.18	0.40	0.51	0.13	0.06	0.88	0.15	0.05	0.09	0.14	0.07	0.90	0.90	0.77	0.31	0.49	4.81	0.46	1.07	2.14	2.43	0.62	0.76	2.45	0.04	0.46	0.27	0.96	0.98	nd	nd	nd	nd
2007-0025	0.16	0.13	0.29	0.55	0.10	0.05	0.95	0.16	0.04	0.09	0.11	0.07	0.92	1.01	0.63	0.31	0.59	4.02	0.37	1.09	2.09	2.51	0.65	0.81	2.92	0.05	0.43	0.23	0.94	0.95	nd	nd	nd	nd
2007-0063	0.20	0.16	0.36	0.51	0.11	0.04	0.87	0.15	0.05	0.09	0.13	0.07	0.98	0.92	0.73	0.31	0.51	4.00	0.44	1.02	2.17	2.43	0.64	0.77	2.67	0.03	0.46	0.28	0.97	0.93	1.62	0.40	1.00	0.88
2007-0064	0.22	0.17	0.39	0.54	0.12	0.04	0.95	0.16	0.05	0.09	0.13	0.08	0.93	0.96	0.74	0.32	0.50	4.17	0.43	1.03	2.14	2.44	0.63	0.78	2.70	0.05	0.46	0.28	0.96	0.92	1.62	0.40	0.89	0.82
2007-0065	0.19	0.15	0.34	0.57	0.10	0.03	1.02	0.17	0.04	0.09	0.11	0.08	0.96	1.01	0.68	0.32	0.55	4.13	0.36	1.12	2.14	2.48	0.65	0.82	3.12	0.05	0.45	0.26	0.95	0.91	1.55	0.37	0.92	0.60
2007-0066	0.18	0.14	0.31	0.57	0.11	0.05	0.95	0.16	0.04	0.09	0.11	0.07	0.84	0.95	0.65	0.33	0.56	3.70	0.40	1.11	2.08	2.39	0.64	0.81	3.72	0.03	0.45	0.26	0.96	0.91	nd	0.26	0.72	0.38
2007-0067	0.18	0.14	0.32	0.56	0.11	0.05	0.94	0.17	0.04	0.09	0.12	0.07	0.89	1.02	0.64	0.32	0.58	3.71	0.34	1.11	2.11	2.44	0.65	0.82	3.33	0.03	0.45	0.27	0.97	0.91	1.53	0.32	0.81	0.50
2007-0068	0.17	0.14	0.31	0.54	0.10	0.05	0.92	0.15	0.04	0.09	0.11	0.07	0.88	1.05	0.64	0.33	0.57	2.95	0.43	1.05	2.12	2.57	0.65	0.83	3.37	0.05	0.44	0.25	0.96	0.90	1.28	0.28	0.78	0.46
2007-0062	0.09	0.11	0.20	0.61	0.04	0.04	0.75	0.16	0.04	0.02	0.08	0.06	0.97	1.06	0.51	0.33	0.70	0.99	0.40	0.79	2.20	2.94	0.29	0.37	1.87	0.05	0.59	0.31	0.97	0.88	1.80	0.18	0.66	0.54
2007-0062a	0.10	0.11	0.22	0.62	0.05	0.04	0.79	0.16	0.04	0.02	0.08	0.06	0.91	1.11	0.54	0.33	0.67	1.01	0.21	0.80	2.19	3.00	0.30	0.38	1.94	0.05	0.60	0.30	0.95	0.88	nd	nd	nd	0.00
2007-0070	0.09	0.11	0.20	0.62	0.04	0.04	0.74	0.16	0.04	0.02	0.09	0.06	1.00	1.08	0.54	0.33	0.66	1.08	0.39	0.80	2.23	3.01	0.28	0.37	1.50	0.05	0.59	0.29	0.98	0.89	nd	nd	nd	0.00
2007-0084	0.16	0.14	0.30	0.55	0.10	0.05	0.91	0.16	0.04	0.08	0.11	0.08	0.94	1.07	0.69	0.31	0.56	3.45	0.43	1.09	2.14	2.45	0.64	0.79	2.39	0.03	0.48	0.29	0.95	0.91	1.63	0.38	0.95	0.80
2007-0105	0.14	0.14	0.28	0.28	0.06	0.07	0.84	0.13	0.05	0.03	0.06	0.07	0.86	0.91	0.67	0.38	0.48	1.71	1.06	1.22	2.33	2.71	0.22	0.30	1.92	0.06	0.43	0.15	0.98	0.91	nd	nd	nd	nd
2007-0282	0.22	0.18	0.40	0.48	0.05	0.04	0.87	0.15	0.04	0.10	0.13	0.08	0.97	1.14	0.73	0.32	0.51	4.44	0.42	1.06	2.21	2.47	0.65	0.78	2.43	0.04	0.44	0.29	0.97	0.90	1.86	1.27	0.10	0.27
2007-0394	0.23	0.18	0.41	0.52	0.11	0.04	0.91	0.16	0.04	0.09	0.13	0.07	0.94	1.11	0.70	0.33	0.52	3.29	0.42	1.05	2.02	2.40	0.66	0.82	2.46	0.04	0.49	0.28	1.00	0.94	2.09	0.45	1.02	0.82
2007-0395	0.23	0.18	0.41	0.55	0.10	0.06	0.96	0.16	0.05	0.10	0.14	0.07	0.91	1.14	0.73	0.31	0.53	3.71	0.35	1.12	2.14	2.33	0.70	0.86	2.79	0.04	0.43	0.25	0.97	0.91	1.74	0.40	0.99	0.65
2007-0017	0.24	0.19	0.42	0.49	0.10	0.06	0.88	0.15	0.04	0.09	0.13	0.07	1.00	1.02	0.72	0.32	0.51	4.64	0.44	1.06	2.18	2.49	0.65	0.80	2.53	0.04	0.45	0.27	0.96	0.96	2.04	0.45	1.11	0.86
2007-0062b	0.11	0.12	0.23	0.66	0.00	0.04	0.80	0.17	0.04	0.01	0.10	0.06	0.95	1.10	0.52	0.34	0.68	0.60	0.18	0.74	2.27	2.98	0.31	0.38	1.73	0.05	0.60	0.33	0.98	0.88	1.65	0.18	0.73	0.56
2007-0070	0.10	0.11	0.21	0.67	0.00	0.04	0.82	0.17	0.05	0.02	0.09	0.06	0.91	1.07	0.53	0.34	0.66	0.47	0.41	0.73	2.25	2.93	0.31	0.40	1.41	0.06	0.56	0.28	0.95	0.91	nd	nd	nd	0.00
2007-0105a	0.15	0.15	0.30	0.30	0.00	0.08	0.82	0.12	0.05	0.03	0.08	0.07	1.00	0.90	0.63	0.39	0.50	1.66	0.96	1.18	2.28	2.67	0.22	0.31	1.93	0.04	0.42	0.24	0.97	0.88	nd	nd	nd	0.00
2007-0014	0.09	0.08	0.17	0.65	0.05	0.03	1.05	0.17	0.03	0.12	0.09	0.08	0.86	1.08	0.50	0.32	0.73	1.67	0.39	1.18	2.02	2.82	0.58	0.78	2.79	0.05	0.45	0.25	0.90	0.87	nd	nd	nd	0.00

*Note: number 1...34 represents the diagnostic ratio name i.e. C28tricycllics, C29 tricyclics, C28+C29tricyclics, 27Ts 28ab 25nor30ab, 29ab 29Ts, 30d, 30O, 30G, 29ba 29aaS, 29bb, 27bbSTER, 28bbSTER, 29bbSTER, TA21, TA26, TA27, 2-MP/1-MP, 4-MD/1-MD C2-dbt/C2-phe, C3-dbt/C3-phe, C3-dbt/C3-chr, Retene/C4-phe, B(a)F/4-Mpy, B(b+c)F/4-Mpy, 2Mpy/4-Mpy, 1Mpy/4-Mpy, DR- SES1/SES2, DR-SES3/SES5, DR- SES4/SES6, DR-SES5/SES10

D

EVALUATION OF DIAGNOSTIC RATIO (CEN METHOD): "FULL CITY" CASE

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0472 Test Date: 03-Sep-2009 Description: Oddane in Vestfold:sand / stones contaminated with oil

Ratio Name	Spill	Mean			Absolute Difference			Critical Difference			Percentage Difference			Flag*		
		R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3
DR-C28 **m/z191**	0.093	0.05	0.09	0.09	0.09	0.00	0.00	0.01	0.01	0.01	200.0	1.5	0.0	0	1	1
DR-C29	0.093	0.05	0.09	0.09	0.09	0.01	0.00	0.01	0.01	0.01	200.0	8.2	0.0	0	1	1
DR-C28C29	0.186	0.09	0.18	0.19	0.19	0.01	0.00	0.01	0.03	0.03	200.0	4.8	0.0	0	1	1
DR-27Ts	0.521	0.50	0.43	0.52	0.04	0.18	0.00	0.07	0.06	0.07	7.5	40.7	0.0	1	0	1
DR-28ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-25nor30ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-29Ts	0.150	0.14	0.13	0.15	0.02	0.03	0.00	0.02	0.02	0.02	11.9	24.1	0.0	1	0	1
DR-30O	0.031	0.04	0.07	0.03	0.02	0.09	0.00	0.01	0.01	0.00	47.6	117.2	0.0	0	0	1
DR-30G	0.097	0.05	0.05	0.10	0.10	0.10	0.00	0.01	0.01	0.01	200.0	200.0	0.0	0	0	1
DR-29ab	0.731	0.72	0.78	0.73	0.02	0.09	0.00	0.10	0.11	0.10	2.9	11.5	0.0	1	1	1
DR-30d	0.049	0.04	0.04	0.05	0.01	0.01	0.00	0.01	0.01	0.01	21.2	26.1	0.0	0	0	1
DR-29aaS **m/z217**	0.975	0.93	0.91	0.98	0.08	0.13	0.00	0.13	0.13	0.14	8.7	14.2	0.0	1	0	1
DR-29bb **&218**	1.083	NaN	1.08	1.08	NaN	0.01	0.00	NaN	0.15	0.15	NaN	0.8	0.0	0	1	1
DR-27bbSTER	0.508	0.51	0.52	0.51	0.01	0.02	0.00	0.07	0.07	0.07	1.7	4.8	0.0	1	1	1
DR-28bbSTER	0.366	0.37	0.36	0.37	0.01	0.01	0.00	0.05	0.05	0.05	2.9	2.7	0.0	1	1	1
DR-29bbSTER	0.654	0.64	0.65	0.65	0.02	0.01	0.00	0.09	0.09	0.09	3.7	2.3	0.0	1	1	1
DR-TA21 **m/z231**	0.451	0.49	0.62	0.45	0.08	0.35	0.00	0.07	0.09	0.06	15.6	55.8	0.0	0	0	1
DR-TA26	0.477	0.45	0.50	0.48	0.04	0.04	0.00	0.06	0.07	0.07	9.5	8.0	0.0	1	1	1
DR-TA27	0.875	0.90	0.90	0.87	0.04	0.06	0.00	0.13	0.13	0.12	4.7	6.4	0.0	1	1	1
DR-2MP/1MP **PAH**	1.893	2.01	2.05	1.89	0.23	0.31	0.00	0.28	0.29	0.27	11.3	14.9	0.0	1	0	1
DR-4MD/1MD	2.542	2.56	2.64	2.54	0.03	0.21	0.00	0.36	0.37	0.36	1.2	7.8	0.0	1	1	1
DR-C2dbt/C2phe	0.396	0.39	0.38	0.40	0.00	0.04	0.00	0.06	0.05	0.06	0.6	9.6	0.0	1	1	1
DR-C3dbt/C3phe	0.602	0.56	0.55	0.60	0.08	0.10	0.00	0.08	0.08	0.08	13.3	18.2	0.0	1	0	1
DR-C3dbt/C3chr	2.391	2.38	2.29	2.39	0.03	0.20	0.00	0.33	0.32	0.33	1.2	8.8	0.0	1	1	1
DR-Retene/C4phe	0.025	0.01	0.05	0.02	0.02	0.04	0.00	0.00	0.01	0.00	200.0	89.9	0.0	0	0	1
DR-BaF/4Mpy	0.461	0.43	0.39	0.46	0.07	0.14	0.00	0.06	0.05	0.06	15.7	34.6	0.0	0	0	1
DR-BbcF/4Mpy	0.244	0.22	0.21	0.24	0.04	0.07	0.00	0.03	0.03	0.03	19.8	32.7	0.0	0	0	1
DR-2Mpy/4Mpy	1.021	1.04	1.08	1.02	0.04	0.11	0.00	0.15	0.15	0.14	3.7	10.1	0.0	1	1	1
DR-1Mpy/4Mpy	0.912	0.91	0.92	0.91	0.00	0.02	0.00	0.13	0.13	0.13	0.1	2.5	0.0	1	1	1
DR-SES1/SES2 **m/z123**	2.314	1.16	2.16	2.31	2.31	0.30	0.00	0.16	0.30	0.32	200.0	14.0	0.0	0	0	1
DR-SES3/SES5	0.331	0.17	0.35	0.33	0.33	0.04	0.00	0.02	0.05	0.05	200.0	12.3	0.0	0	1	1
DR-SES4/SES6	0.832	0.42	0.92	0.83	0.83	0.18	0.00	0.06	0.13	0.12	200.0	19.5	0.0	0	0	1
DR-SES5/SES10	0.729	0.36	0.95	0.73	0.73	0.44	0.00	0.05	0.13	0.10	200.0	46.1	0.0	0	0	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	**Test Date**	**Sample Description**
1. 2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.1: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0472) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0485 Test Date: 03-Sep-2009 Description: Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn

Ratio Name	Spill	Mean			Absolute Difference			Critical Difference			Percentage Difference			Flag*		
		R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3
DR-C28 **m/z191**	0.091	0.05	0.09	0.09	0.09	0.00	0.00	0.01	0.01	0.01	200.0	0.0	1.5	0	1	1
DR-C29	0.086	0.04	0.09	0.09	0.09	0.00	0.01	0.01	0.01	0.01	200.0	0.0	8.2	0	1	1
DR-C28C29	0.177	0.09	0.18	0.18	0.18	0.00	0.01	0.01	0.02	0.03	200.0	0.0	4.8	0	1	1
DR-27Ts	0.345	0.41	0.34	0.43	0.14	0.00	0.18	0.06	0.05	0.06	33.5	0.0	40.7	0	1	0
DR-28ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-25nor30ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-29Ts	0.118	0.13	0.12	0.13	0.02	0.00	0.03	0.02	0.02	0.02	12.3	0.0	24.1	1	1	0
DR-30O	0.118	0.08	0.12	0.07	0.07	0.00	0.09	0.01	0.02	0.01	80.9	0.0	117.2	0	1	0
DR-30G	0.000	0.00	0.00	0.05	0.00	0.00	0.10	0.00	0.00	0.01	NaN	NaN	200.0	0	0	0
DR-29ab	0.820	0.76	0.82	0.78	0.11	0.00	0.09	0.11	0.11	0.11	14.3	0.0	11.5	0	1	1
DR-30d	0.038	0.04	0.04	0.04	0.00	0.00	0.01	0.01	0.01	0.01	4.9	0.0	26.1	1	1	0
DR-29aaS **m/z217**	0.846	0.87	0.85	0.91	0.05	0.00	0.13	0.12	0.12	0.13	5.5	0.0	14.2	1	1	0
DR-29bb **&218**	1.074	NaN	1.07	1.08	NaN	0.00	0.01	NaN	0.15	0.15	NaN	0.0	0.8	0	1	1
DR-27bbSTER	0.533	0.52	0.53	0.52	0.02	0.00	0.02	0.07	0.07	0.07	3.1	0.0	4.8	1	1	1
DR-28bbSTER	0.356	0.37	0.36	0.36	0.02	0.00	0.01	0.05	0.05	0.05	5.6	0.0	2.7	1	1	1
DR-29bbSTER	0.639	0.63	0.64	0.65	0.01	0.00	0.01	0.09	0.09	0.09	1.4	0.0	2.3	1	1	1
DR-TA21 **m/z231**	0.799	0.66	0.80	0.62	0.27	0.00	0.35	0.09	0.11	0.09	41.1	0.0	55.8	0	1	0
DR-TA26	0.516	0.47	0.52	0.50	0.08	0.00	0.04	0.07	0.07	0.07	17.5	0.0	8.0	0	1	1
DR-TA27	0.933	0.92	0.93	0.90	0.02	0.00	0.06	0.13	0.13	0.13	1.7	0.0	6.4	1	1	1
DR-2MP/1MP **PAH**	2.198	2.16	2.20	2.05	0.08	0.00	0.31	0.30	0.31	0.29	3.6	0.0	14.9	1	1	0
DR-4MD/1MD	2.747	2.66	2.75	2.64	0.17	0.00	0.21	0.37	0.38	0.37	6.5	0.0	7.8	1	1	1
DR-C2dbt/C2phe	0.360	0.38	0.36	0.38	0.03	0.00	0.04	0.05	0.05	0.05	9.0	0.0	9.6	1	1	1
DR-C3dbt/C3phe	0.502	0.51	0.50	0.55	0.02	0.00	0.10	0.07	0.07	0.08	4.9	0.0	18.2	1	1	0
DR-C3dbt/C3chr	2.189	2.28	2.19	2.29	0.17	0.00	0.20	0.32	0.31	0.32	7.6	0.0	8.8	1	1	1
DR-Retene/C4phe	0.065	0.03	0.07	0.05	0.07	0.00	0.04	0.00	0.01	0.01	200.0	0.0	89.9	0	1	0
DR-BaF/4Mpy	0.325	0.36	0.32	0.39	0.07	0.00	0.14	0.05	0.05	0.05	19.1	0.0	34.6	0	1	0
DR-BbcF/4Mpy	0.175	0.19	0.18	0.21	0.02	0.00	0.07	0.03	0.02	0.03	13.1	0.0	32.7	1	1	0
DR-2Mpy/4Mpy	1.130	1.09	1.13	1.08	0.07	0.00	0.11	0.15	0.16	0.15	6.4	0.0	10.1	1	1	1
DR-1Mpy/4Mpy	0.936	0.92	0.94	0.92	0.02	0.00	0.02	0.13	0.13	0.13	2.4	0.0	2.5	1	1	1
DR-SES1/SES2 **m/z123**	2.010	1.01	2.01	2.16	2.01	0.00	0.30	0.14	0.28	0.30	200.0	0.0	14.0	0	1	0
DR-SES3/SES5	0.374	0.19	0.37	0.35	0.37	0.00	0.04	0.03	0.05	0.05	200.0	0.0	12.3	0	1	1
DR-SES4/SES6	1.012	0.51	1.01	0.92	1.01	0.00	0.18	0.07	0.14	0.13	200.0	0.0	19.5	0	1	0
DR-SES5/SES10	1.167	0.58	1.17	0.95	1.17	0.00	0.44	0.08	0.16	0.13	200.0	0.0	46.1	0	1	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.2: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0485) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0486 Test Date: 03-Sep-2009 Description: Landoy/Mandal:Oil w / traces of free water

Ratio Name	Spill	Mean			Absolute Difference			Critical Difference			Percentage Difference			Flag*		
		R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3
DR-C28 **m/z191**	0.087	0.04	0.09	0.09	0.09	0.00	0.01	0.01	0.01	0.01	200.0	4.6	6.1	0	1	1
DR-C29	0.090	0.04	0.09	0.09	0.09	0.00	0.00	0.01	0.01	0.01	200.0	4.5	3.7	0	1	1
DR-C28C29	0.177	0.09	0.18	0.18	0.18	0.00	0.01	0.01	0.02	0.03	200.0	0.1	4.9	0	1	1
DR-27Ts	0.499	0.49	0.42	0.51	0.02	0.15	0.02	0.07	0.06	0.07	3.1	36.5	4.4	1	0	1
DR-28ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-25nor30ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-29Ts	0.143	0.14	0.13	0.15	0.01	0.03	0.01	0.02	0.02	0.02	7.3	19.5	4.7	1	0	1
DR-30O	0.045	0.05	0.08	0.04	0.01	0.07	0.01	0.01	0.01	0.01	11.0	89.9	37.1	1	0	0
DR-30G	0.090	0.04	0.04	0.09	0.09	0.09	0.01	0.01	0.01	0.01	200.0	200.0	8.2	0	0	1
DR-29ab	0.725	0.72	0.77	0.73	0.02	0.09	0.01	0.10	0.11	0.10	2.1	12.2	0.8	1	1	1
DR-30d	0.046	0.04	0.04	0.05	0.01	0.01	0.00	0.01	0.01	0.01	14.8	19.7	6.5	0	0	1
DR-29aaS **m/z217**	0.961	0.93	0.90	0.97	0.07	0.12	0.01	0.13	0.13	0.14	7.3	12.8	1.4	1	1	1
DR-29bb **&218**	1.070	NaN	1.07	1.08	NaN	0.00	0.01	NaN	0.15	0.15	NaN	0.4	1.2	0	1	1
DR-27bbSTER	0.529	0.52	0.53	0.52	0.01	0.00	0.02	0.07	0.07	0.07	2.4	0.6	4.2	1	1	1
DR-28bbSTER	0.369	0.37	0.36	0.37	0.01	0.01	0.00	0.05	0.05	0.05	2.0	3.6	0.9	1	1	1
DR-29bbSTER	0.624	0.63	0.63	0.64	0.01	0.01	0.03	0.09	0.09	0.09	0.9	2.3	4.6	1	1	1
DR-TA21 **m/z231**	0.486	0.51	0.64	0.47	0.04	0.31	0.04	0.07	0.09	0.07	8.0	48.7	7.6	1	0	1
DR-TA26	0.450	0.44	0.48	0.46	0.02	0.07	0.03	0.06	0.07	0.06	3.7	13.8	5.8	1	1	1
DR-TA27	0.867	0.89	0.90	0.87	0.05	0.07	0.01	0.12	0.13	0.12	5.6	7.3	0.9	1	1	1
DR-2MP/1MP **PAH**	2.000	2.06	2.10	1.95	0.12	0.20	0.11	0.29	0.29	0.27	5.8	9.4	5.5	1	1	1
DR-4MD/1MD	2.534	2.55	2.64	2.54	0.04	0.21	0.01	0.36	0.37	0.36	1.5	8.1	0.3	1	1	1
DR-C2dbt/C2phe	0.385	0.39	0.37	0.39	0.01	0.03	0.01	0.05	0.05	0.05	2.2	6.8	2.8	1	1	1
DR-C3dbt/C3phe	0.556	0.54	0.53	0.58	0.03	0.05	0.05	0.08	0.07	0.08	5.4	10.2	8.0	1	1	1
DR-C3dbt/C3chr	2.420	2.39	2.30	2.41	0.06	0.23	0.03	0.33	0.32	0.34	2.4	10.0	1.2	1	1	1
DR-Retene/C4phe	0.021	0.01	0.04	0.02	0.02	0.04	0.00	0.00	0.01	0.00	200.0	103.3	17.4	0	0	0
DR-BaF/4Mpy	0.394	0.39	0.36	0.43	0.00	0.07	0.07	0.06	0.05	0.06	0.2	19.2	15.6	1	0	0
DR-BbcF/4Mpy	0.187	0.19	0.18	0.22	0.01	0.01	0.06	0.03	0.03	0.03	6.9	6.2	26.6	1	1	0
DR-2Mpy/4Mpy	1.052	1.06	1.09	1.04	0.01	0.08	0.03	0.15	0.15	0.15	0.7	7.1	3.0	1	1	1
DR-1Mpy/4Mpy	0.897	0.91	0.92	0.90	0.02	0.04	0.01	0.13	0.13	0.13	1.8	4.2	1.7	1	1	1
DR-SES1/SES2 **m/z123**	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0
DR-SES3/SES5	0.277	0.14	0.33	0.30	0.28	0.10	0.05	0.02	0.05	0.04	200.0	29.8	17.7	0	0	0
DR-SES4/SES6	0.757	0.38	0.88	0.79	0.76	0.26	0.08	0.05	0.12	0.11	200.0	28.8	9.5	0	0	1
DR-SES5/SES10	0.674	0.34	0.92	0.70	0.67	0.49	0.05	0.05	0.13	0.10	200.0	53.5	7.8	0	0	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.3: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0486) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0489 Test Date: 03-Sep-2009 Description: Barge by unloading:Sample 21, taken by E. Lydersen, saksnr. 108-27053

Ratio Name		Spill	Mean			Absolute Difference			Critical Difference			Percentage Difference			Flag*		
			R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3
DR-C28	**m/z191**	0.080	0.04	0.09	0.09	0.08	0.01	0.01	0.01	0.01	0.01	200.0	13.3	14.8	0	1	0
DR-C29		0.110	0.05	0.10	0.10	0.11	0.02	0.02	0.01	0.01	0.01	200.0	24.7	16.6	0	0	0
DR-C28C29		0.190	0.09	0.18	0.19	0.19	0.01	0.00	0.01	0.03	0.03	200.0	7.0	2.2	0	1	1
DR-27Ts		0.617	0.55	0.48	0.57	0.13	0.27	0.10	0.08	0.07	0.08	24.3	56.6	16.9	0	0	0
DR-28ab		0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-25nor30ab		0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-29Ts		0.159	0.15	0.14	0.15	0.03	0.04	0.01	0.02	0.02	0.02	17.7	29.8	5.8	0	0	1
DR-30O		0.000	0.02	0.06	0.02	0.05	0.12	0.03	0.00	0.01	0.00	200.0	200.0	200.0	0	0	0
DR-30G		0.095	0.05	0.05	0.10	0.10	0.10	0.00	0.01	0.01	0.01	200.0	200.0	2.4	0	0	1
DR-29ab		0.701	0.71	0.76	0.72	0.01	0.12	0.03	0.10	0.11	0.10	1.3	15.7	4.2	1	0	1
DR-30d		0.047	0.04	0.04	0.05	0.01	0.01	0.00	0.01	0.01	0.01	15.1	20.0	6.1	0	0	1
DR-29aaS	**m/z217**	0.983	0.94	0.91	0.98	0.09	0.14	0.01	0.13	0.13	0.14	9.6	15.0	0.9	1	0	1
DR-29bb	**&218**	1.055	NaN	1.06	1.07	NaN	0.02	0.03	NaN	0.15	0.15	NaN	1.8	2.6	0	1	1
DR-27bbSTER		0.509	0.51	0.52	0.51	0.01	0.02	0.00	0.07	0.07	0.07	1.4	4.5	0.3	1	1	1
DR-28bbSTER		0.365	0.37	0.36	0.37	0.01	0.01	0.00	0.05	0.05	0.05	3.0	2.6	0.1	1	1	1
DR-29bbSTER		0.653	0.64	0.65	0.65	0.02	0.01	0.00	0.09	0.09	0.09	3.5	2.1	0.2	1	1	1
DR-TA21	**m/z231**	0.397	0.46	0.60	0.42	0.13	0.40	0.05	0.06	0.08	0.06	28.0	67.2	12.6	0	0	1
DR-TA26		0.446	0.44	0.48	0.46	0.01	0.07	0.03	0.06	0.07	0.06	2.9	14.6	6.6	1	0	1
DR-TA27		0.852	0.88	0.89	0.86	0.07	0.08	0.02	0.12	0.12	0.12	7.4	9.1	2.7	1	1	1
DR-2MP/1MP	**PAH**	1.418	1.77	1.81	1.66	0.70	0.78	0.47	0.25	0.25	0.23	39.7	43.1	28.7	0	0	0
DR-4MD/1MD		2.157	2.37	2.45	2.35	0.42	0.59	0.39	0.33	0.34	0.33	17.6	24.1	16.4	0	0	0
DR-C2dbt/C2phe		0.508	0.45	0.43	0.45	0.11	0.15	0.11	0.06	0.06	0.06	25.5	34.2	24.8	0	0	0
DR-C3dbt/C3phe		0.632	0.58	0.57	0.62	0.11	0.13	0.03	0.08	0.08	0.09	18.2	23.0	4.9	0	0	1
DR-C3dbt/C3chr		2.027	2.20	2.11	2.21	0.34	0.16	0.36	0.31	0.30	0.31	15.3	7.7	16.5	0	1	0
DR-Retene/C4phe		0.041	0.02	0.05	0.03	0.04	0.02	0.02	0.00	0.01	0.00	200.0	46.5	48.5	0	0	0
DR-BaF/4Mpy		0.919	0.66	0.62	0.69	0.53	0.59	0.46	0.09	0.09	0.10	80.1	95.5	66.5	0	0	0
DR-BbcF/4Mpy		0.431	0.32	0.30	0.34	0.23	0.26	0.19	0.04	0.04	0.05	73.2	84.2	55.4	0	0	0
DR-2Mpy/4Mpy		0.795	0.93	0.96	0.91	0.27	0.34	0.23	0.13	0.13	0.13	28.6	34.8	25.0	0	0	0
DR-1Mpy/4Mpy		0.862	0.89	0.90	0.89	0.05	0.07	0.05	0.12	0.13	0.12	5.8	8.2	5.7	1	1	1
DR-SES1/SES2	**m/z123**	1.823	0.91	1.92	2.07	1.82	0.19	0.49	0.13	0.27	0.29	200.0	9.8	23.7	0	1	0
DR-SES3/SES5		0.413	0.21	0.39	0.37	0.41	0.04	0.08	0.03	0.06	0.05	200.0	10.0	22.2	0	1	0
DR-SES4/SES6		0.975	0.49	0.99	0.90	0.98	0.04	0.14	0.07	0.14	0.13	200.0	3.7	15.8	0	1	0
DR-SES5/SES10		0.720	0.36	0.94	0.72	0.72	0.45	0.01	0.05	0.13	0.10	200.0	47.4	1.3	0	0	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.4: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0489) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009–0491 Test Date: 03–Sep–2009 Description: Nevlunghavn, Ødegårdsfjord:1–15 mm thick, taken in Steinvik in 0degårdsfjord, Nevlunghavn

Ratio Name		Spill	Mean			Absolute Difference			Critical Difference			Percentage Difference			Flag*		
			R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3
DR–C28	**m/z191**	0.083	0.04	0.09	0.09	0.08	0.01	0.01	0.01	0.01	0.01	200.0	9.8	11.3	0	1	1
DR–C29		0.124	0.06	0.10	0.11	0.12	0.04	0.03	0.01	0.01	0.02	200.0	36.3	28.3	0	0	0
DR–C28C29		0.206	0.10	0.19	0.20	0.21	0.03	0.02	0.01	0.03	0.03	200.0	15.4	10.6	0	0	1
DR–27Ts		0.447	0.46	0.40	0.48	0.04	0.10	0.07	0.07	0.06	0.07	7.9	25.7	15.4	1	0	0
DR–28ab		0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR–25nor30ab		0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR–29Ts		0.137	0.14	0.13	0.14	0.00	0.02	0.01	0.02	0.02	0.02	2.9	15.2	9.0	1	0	1
DR–30O		0.066	0.06	0.09	0.05	0.02	0.05	0.04	0.01	0.01	0.01	27.3	56.7	72.6	0	0	0
DR–30G		0.086	0.04	0.04	0.09	0.09	0.09	0.01	0.01	0.01	0.01	200.0	200.0	12.9	0	0	1
DR–29ab		0.752	0.73	0.79	0.74	0.04	0.07	0.02	0.10	0.11	0.10	5.7	8.6	2.8	1	1	1
DR–30d		0.043	0.04	0.04	0.05	0.00	0.00	0.01	0.01	0.01	0.01	6.7	11.6	14.5	1	1	0
DR–29aaS	**m/z217**	0.933	0.91	0.89	0.95	0.04	0.09	0.04	0.13	0.12	0.13	4.4	9.8	4.4	1	1	1
DR–29bb	**&218**	1.057	NaN	1.07	1.07	NaN	0.02	0.03	NaN	0.15	0.15	NaN	1.6	2.5	0	1	1
DR–27bbSTER		0.519	0.52	0.53	0.51	0.00	0.01	0.01	0.07	0.07	0.07	0.4	2.6	2.2	1	1	1
DR–28bbSTER		0.374	0.38	0.36	0.37	0.00	0.02	0.01	0.05	0.05	0.05	0.8	4.8	2.1	1	1	1
DR–29bbSTER		0.629	0.63	0.63	0.64	0.00	0.01	0.02	0.09	0.09	0.09	0.1	1.5	3.8	1	1	1
DR–TA21	**m/z231**	0.534	0.53	0.67	0.49	0.01	0.26	0.08	0.07	0.09	0.07	1.5	39.7	17.1	1	0	0
DR–TA26		0.462	0.45	0.49	0.47	0.03	0.05	0.02	0.06	0.07	0.07	6.3	11.2	3.2	1	1	1
DR–TA27		0.862	0.89	0.90	0.87	0.05	0.07	0.01	0.12	0.13	0.12	6.2	7.9	1.5	1	1	1
DR–2MP/1MP	**PAH**	1.988	2.05	2.09	1.94	0.13	0.21	0.10	0.29	0.29	0.27	6.4	10.0	4.9	1	1	1
DR–4MD/1MD		2.666	2.62	2.71	2.60	0.09	0.08	0.12	0.37	0.38	0.36	3.5	3.0	4.7	1	1	1
DR–C2dbt/C2phe		0.384	0.39	0.37	0.39	0.01	0.02	0.01	0.05	0.05	0.05	2.5	6.4	3.2	1	1	1
DR–C3dbt/C3phe		0.514	0.52	0.51	0.56	0.01	0.01	0.09	0.07	0.07	0.08	2.5	2.3	15.9	1	1	0
DR–C3dbt/C3chr		2.258	2.31	2.22	2.32	0.10	0.07	0.13	0.32	0.31	0.33	4.5	3.1	5.7	1	1	1
DR–Retene/C4phe		0.017	0.01	0.04	0.02	0.02	0.05	0.01	0.00	0.01	0.00	200.0	117.5	37.5	0	0	0
DR–BaF/4Mpy		0.354	0.37	0.34	0.41	0.04	0.03	0.11	0.05	0.05	0.06	10.4	8.7	26.1	1	1	0
DR–BbcF/4Mpy		0.194	0.20	0.18	0.22	0.01	0.02	0.05	0.03	0.03	0.03	3.2	9.9	23.0	1	1	0
DR–2Mpy/4Mpy		1.081	1.07	1.11	1.05	0.02	0.05	0.06	0.15	0.15	0.15	1.9	4.4	5.7	1	1	1
DR–1Mpy/4Mpy		0.914	0.91	0.92	0.91	0.00	0.02	0.00	0.13	0.13	0.13	0.1	2.3	0.2	1	1	1
DR–SES1/SES2	**m/z123**	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0
DR–SES3/SES5		0.273	0.14	0.32	0.30	0.27	0.10	0.06	0.02	0.05	0.04	200.0	31.1	19.0	0	0	0
DR–SES4/SES6		0.769	0.38	0.89	0.80	0.77	0.24	0.06	0.05	0.12	0.11	200.0	27.3	7.9	0	0	1
DR–SES5/SES10		0.689	0.34	0.93	0.71	0.69	0.48	0.04	0.05	0.13	0.10	200.0	51.5	5.8	0	0	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2009–0579	Aug–2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009–0485	03–Sep–2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009–0472	03–Sep–2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.5: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0491) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0493 Test Date: 03-Sep-2009 Description: Langesund Bad:Langesund bad, 1 mm. Krogshavn.

Ratio Name		Spill	Mean			Absolute Difference			Critical Difference			Percentage Difference			Flag*		
			R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3
DR-C28	**m/z191**	0.083	0.04	0.09	0.09	0.08	0.01	0.01	0.01	0.01	0.01	200.0	9.5	11.0	0	1	1
DR-C29		0.185	0.09	0.14	0.14	0.19	0.10	0.09	0.01	0.02	0.02	200.0	73.6	66.4	0	0	0
DR-C28C29		0.268	0.13	0.22	0.23	0.27	0.09	0.08	0.02	0.03	0.03	200.0	41.1	36.5	0	0	0
DR-27Ts		0.336	0.41	0.34	0.43	0.15	0.01	0.18	0.06	0.05	0.06	35.9	2.5	43.1	0	1	0
DR-28ab		0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-25nor30ab		0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-29Ts		0.126	0.13	0.12	0.14	0.01	0.01	0.02	0.02	0.02	0.02	5.3	7.0	17.2	1	1	0
DR-30O		0.127	0.09	0.12	0.08	0.08	0.01	0.10	0.01	0.02	0.01	87.1	7.5	122.1	0	1	0
DR-30G		0.083	0.04	0.04	0.09	0.08	0.08	0.01	0.01	0.01	0.01	200.0	200.0	16.3	0	0	0
DR-29ab		0.798	0.75	0.81	0.76	0.09	0.02	0.07	0.11	0.11	0.11	11.7	2.7	8.8	1	1	1
DR-30d		0.034	0.04	0.04	0.04	0.01	0.00	0.02	0.01	0.01	0.01	16.6	11.7	37.5	0	1	0
DR-29aaS	**m/z217**	0.846	0.87	0.85	0.91	0.05	0.00	0.13	0.12	0.12	0.13	5.5	0.0	14.2	1	1	0
DR-29bb	**&218**	1.057	NaN	1.07	1.07	NaN	0.02	0.03	NaN	0.15	0.15	NaN	1.6	2.4	0	1	1
DR-27bbSTER		0.516	0.52	0.52	0.51	0.00	0.02	0.01	0.07	0.07	0.07	0.1	3.1	1.7	1	1	1
DR-28bbSTER		0.343	0.36	0.35	0.35	0.03	0.01	0.02	0.05	0.05	0.05	9.4	3.8	6.5	1	1	1
DR-29bbSTER		0.678	0.65	0.66	0.67	0.05	0.04	0.02	0.09	0.09	0.09	7.4	6.0	3.7	1	1	1
DR-TA21	**m/z231**	0.860	0.69	0.83	0.66	0.33	0.06	0.41	0.10	0.12	0.09	48.1	7.4	62.5	0	1	0
DR-TA26		0.485	0.46	0.50	0.48	0.05	0.03	0.01	0.06	0.07	0.07	11.3	6.2	1.8	1	1	1
DR-TA27		0.899	0.91	0.92	0.89	0.02	0.03	0.02	0.13	0.13	0.12	1.9	3.6	2.8	1	1	1
DR-2MP/1MP	**PAH**	1.980	2.05	2.09	1.94	0.14	0.22	0.09	0.29	0.29	0.27	6.8	10.4	4.5	1	1	1
DR-4MD/1MD		2.651	2.61	2.70	2.60	0.08	0.10	0.11	0.37	0.38	0.36	3.0	3.6	4.2	1	1	1
DR-C2dbt/C2phe		0.383	0.39	0.37	0.39	0.01	0.02	0.01	0.05	0.05	0.05	2.5	6.4	3.2	1	1	1
DR-C3dbt/C3phe		0.541	0.53	0.52	0.57	0.01	0.04	0.06	0.07	0.07	0.08	2.7	7.5	10.7	1	1	1
DR-C3dbt/C3chr		2.546	2.45	2.37	2.47	0.18	0.36	0.15	0.34	0.33	0.35	7.4	15.0	6.3	1	0	1
DR-Retene/C4phe		0.038	0.02	0.05	0.03	0.04	0.03	0.01	0.00	0.01	0.00	200.0	51.8	43.1	0	0	0
DR-BaF/4Mpy		0.346	0.37	0.34	0.40	0.05	0.02	0.11	0.05	0.05	0.06	12.9	6.2	28.5	1	1	0
DR-BbcF/4Mpy		0.175	0.19	0.18	0.21	0.02	0.00	0.07	0.03	0.02	0.03	13.1	0.1	32.7	1	1	0
DR-2Mpy/4Mpy		1.130	1.10	1.13	1.08	0.07	0.00	0.11	0.15	0.16	0.15	6.4	0.0	10.1	1	1	1
DR-1Mpy/4Mpy		0.887	0.90	0.91	0.90	0.03	0.05	0.03	0.13	0.13	0.13	2.9	5.3	2.8	1	1	1
DR-SES1/SES2	**m/z123**	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0
DR-SES3/SES5		0.229	0.11	0.30	0.28	0.23	0.15	0.10	0.02	0.04	0.04	200.0	48.2	36.4	0	0	0
DR-SES4/SES6		0.783	0.39	0.90	0.81	0.78	0.23	0.05	0.05	0.13	0.11	200.0	25.6	6.2	0	0	1
DR-SES5/SES10		0.536	0.27	0.85	0.63	0.54	0.63	0.19	0.04	0.12	0.09	200.0	74.0	30.5	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

	SINTEF ID	**Test Date**	**Sample Description**
1.	2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2.	2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3.	2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.6: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0493) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0499 Test Date: 03-Sep-2009 Description: Hassletangen Grimstad:Ruakerkilen outside the entrance.Viscous coating spring stones

Ratio Name	Spill	Mean			Absolute Difference			Critical Difference			Percentage Difference			Flag*		
		R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3
DR-C28 **m/z191**	0.083	0.04	0.09	0.09	0.08	0.01	0.01	0.01	0.01	0.01	200.0	9.5	11.0	0	1	1
DR-C29	0.126	0.06	0.11	0.11	0.13	0.04	0.03	0.01	0.01	0.02	200.0	38.4	30.4	0	0	0
DR-C28C29	0.209	0.10	0.19	0.20	0.21	0.03	0.02	0.01	0.03	0.03	200.0	16.8	12.0	0	0	1
DR-27Ts	0.512	0.50	0.43	0.52	0.03	0.17	0.01	0.07	0.06	0.07	5.8	39.1	1.7	1	0	1
DR-28ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-25nor30ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-29Ts	0.140	0.14	0.13	0.15	0.01	0.02	0.01	0.02	0.02	0.02	5.2	17.5	6.7	1	0	1
DR-30O	0.041	0.05	0.08	0.04	0.01	0.08	0.01	0.01	0.01	0.01	20.3	97.2	28.0	0	0	0
DR-30G	0.090	0.05	0.05	0.09	0.09	0.09	0.01	0.01	0.01	0.01	200.0	200.0	7.8	0	0	1
DR-29ab	0.703	0.71	0.76	0.72	0.01	0.12	0.03	0.10	0.11	0.10	1.0	15.3	3.8	1	0	1
DR-30d	0.043	0.04	0.04	0.05	0.00	0.00	0.01	0.01	0.01	0.01	7.2	12.1	14.1	1	1	0
DR-29aaS **m/z217**	0.923	0.91	0.88	0.95	0.03	0.08	0.05	0.13	0.12	0.13	3.2	8.7	5.5	1	1	1
DR-29bb **&218**	1.018	NaN	1.05	1.05	NaN	0.06	0.06	NaN	0.15	0.15	NaN	5.3	6.2	0	1	1
DR-27bbSTER	0.523	0.52	0.53	0.52	0.01	0.01	0.02	0.07	0.07	0.07	1.3	1.8	3.0	1	1	1
DR-28bbSTER	0.369	0.37	0.36	0.37	0.01	0.01	0.00	0.05	0.05	0.05	2.2	3.4	0.7	1	1	1
DR-29bbSTER	0.631	0.63	0.64	0.64	0.00	0.01	0.02	0.09	0.09	0.09	0.2	1.2	3.5	1	1	1
DR-TA21 **m/z231**	0.486	0.51	0.64	0.47	0.04	0.31	0.04	0.07	0.09	0.07	8.0	48.7	7.6	1	0	1
DR-TA26	0.460	0.45	0.49	0.47	0.03	0.06	0.02	0.06	0.07	0.07	5.9	11.6	3.6	1	1	1
DR-TA27	0.852	0.88	0.89	0.86	0.06	0.08	0.02	0.12	0.12	0.12	7.3	9.0	2.6	1	1	1
DR-2MP/1MP **PAH**	1.905	2.01	2.05	1.90	0.22	0.29	0.01	0.28	0.29	0.27	10.7	14.3	0.6	1	0	1
DR-4MD/1MD	2.526	2.55	2.64	2.53	0.05	0.22	0.02	0.36	0.37	0.35	1.9	8.4	0.6	1	1	1
DR-C2dbt/C2phe	0.369	0.38	0.36	0.38	0.02	0.01	0.03	0.05	0.05	0.05	6.3	2.7	6.9	1	1	1
DR-C3dbt/C3phe	0.553	0.54	0.53	0.58	0.03	0.05	0.05	0.08	0.07	0.08	4.9	9.7	8.4	1	1	1
DR-C3dbt/C3chr	2.196	2.28	2.19	2.29	0.17	0.01	0.19	0.32	0.31	0.32	7.3	0.3	8.5	1	1	1
DR-Retene/C4phe	0.023	0.01	0.04	0.02	0.02	0.04	0.00	0.00	0.01	0.00	200.0	97.0	9.1	0	0	1
DR-BaF/4Mpy	0.403	0.40	0.36	0.43	0.01	0.08	0.06	0.06	0.05	0.06	2.5	21.5	13.3	1	0	1
DR-BbcF/4Mpy	0.202	0.20	0.19	0.22	0.00	0.03	0.04	0.03	0.03	0.03	1.2	14.3	18.6	1	0	0
DR-2Mpy/4Mpy	1.045	1.05	1.09	1.03	0.01	0.08	0.02	0.15	0.15	0.14	1.4	7.8	2.3	1	1	1
DR-1Mpy/4Mpy	0.909	0.91	0.92	0.91	0.00	0.03	0.00	0.13	0.13	0.13	0.5	2.9	0.3	1	1	1
DR-SES1/SES2 **m/z123**	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0
DR-SES3/SES5	0.000	0.00	0.19	0.17	0.00	0.37	0.33	0.00	0.03	0.02	NaN	200.0	200.0	0	0	0
DR-SES4/SES6	0.729	0.36	0.87	0.78	0.73	0.28	0.10	0.05	0.12	0.11	200.0	32.6	13.3	0	0	1
DR-SES5/SES10	0.514	0.26	0.84	0.62	0.51	0.65	0.22	0.04	0.12	0.09	200.0	77.6	34.6	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.7: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0499) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0500 Test Date: 03-Sep-2009 Description: Fie v/Risør:Petroleum Lumps(about 5 mL)

Ratio Name		**Spill**	**Mean**			**Absolute Difference**			**Critical Difference**			**Percentage Difference**			**Flag***		
			R1	**R2**	**R3**	**R1**	**R2**	**R3**	**R1**	**R2**	**R3**	**R1**	**R2**	**R3**	**R1**	**R2**	**R3**
DR-C28	**m/z191**	0.084	0.04	0.09	0.09	0.08	0.01	0.01	0.01	0.01	0.01	200.0	8.0	9.5	0	1	1
DR-C29		0.172	0.09	0.13	0.13	0.17	0.09	0.08	0.01	0.02	0.02	200.0	67.0	59.6	0	0	0
DR-C28C29		0.256	0.13	0.22	0.22	0.26	0.08	0.07	0.02	0.03	0.03	200.0	36.6	31.9	0	0	0
DR-27Ts		0.516	0.50	0.43	0.52	0.03	0.17	0.01	0.07	0.06	0.07	6.5	39.8	1.0	1	0	1
DR-28ab		0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-25nor30ab		0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-29Ts		0.146	0.14	0.13	0.15	0.01	0.03	0.00	0.02	0.02	0.02	9.1	21.3	2.9	1	0	1
DR-30O		0.040	0.05	0.08	0.04	0.01	0.08	0.01	0.01	0.01	0.00	21.4	98.1	26.9	0	0	0
DR-30G		0.086	0.04	0.04	0.09	0.09	0.09	0.01	0.01	0.01	0.01	200.0	200.0	12.5	0	0	1
DR-29ab		0.721	0.72	0.77	0.73	0.01	0.10	0.01	0.10	0.11	0.10	1.6	12.8	1.3	1	1	1
DR-30d		0.046	0.04	0.04	0.05	0.01	0.01	0.00	0.01	0.01	0.01	12.9	17.8	8.4	1	0	1
DR-29aaS	**m/z217**	0.984	0.94	0.91	0.98	0.09	0.14	0.01	0.13	0.13	0.14	9.6	15.1	0.9	1	0	1
DR-29bb	**&218**	1.071	NaN	1.07	1.08	NaN	0.00	0.01	NaN	0.15	0.15	NaN	0.3	1.2	0	1	1
DR-27bbSTER		0.493	0.50	0.51	0.50	0.02	0.04	0.01	0.07	0.07	0.07	4.6	7.7	2.9	1	1	1
DR-28bbSTER		0.378	0.38	0.37	0.37	0.00	0.02	0.01	0.05	0.05	0.05	0.3	5.9	3.2	1	1	1
DR-29bbSTER		0.654	0.64	0.65	0.65	0.02	0.02	0.00	0.09	0.09	0.09	3.8	2.4	0.1	1	1	1
DR-TA21	**m/z231**	0.462	0.49	0.63	0.46	0.06	0.34	0.01	0.07	0.09	0.06	13.0	53.4	2.6	1	0	1
DR-TA26		0.439	0.44	0.48	0.46	0.01	0.08	0.04	0.06	0.07	0.06	1.3	16.2	8.2	1	0	1
DR-TA27		0.857	0.89	0.89	0.87	0.06	0.08	0.02	0.12	0.13	0.12	6.7	8.4	2.0	1	1	1
DR-2MP/1MP	**PAH**	1.899	2.01	2.05	1.90	0.22	0.30	0.01	0.28	0.29	0.27	11.0	14.6	0.3	1	0	1
DR-4MD/1MD		2.507	2.54	2.63	2.52	0.07	0.24	0.03	0.36	0.37	0.35	2.6	9.1	1.4	1	1	1
DR-C2dbt/C2phe		0.384	0.39	0.37	0.39	0.01	0.02	0.01	0.05	0.05	0.05	2.4	6.6	3.0	1	1	1
DR-C3dbt/C3phe		0.568	0.55	0.53	0.58	0.04	0.07	0.03	0.08	0.07	0.08	7.5	12.4	5.8	1	1	1
DR-C3dbt/C3chr		2.376	2.37	2.28	2.38	0.01	0.19	0.02	0.33	0.32	0.33	0.5	8.2	0.6	1	1	1
DR-Retene/C4phe		0.024	0.01	0.04	0.02	0.02	0.04	0.00	0.00	0.01	0.00	200.0	93.2	4.2	0	0	1
DR-BaF/4Mpy		0.414	0.40	0.37	0.44	0.02	0.09	0.05	0.06	0.05	0.06	5.0	24.0	10.7	1	0	1
DR-BbcF/4Mpy		0.189	0.19	0.18	0.22	0.01	0.01	0.05	0.03	0.03	0.03	5.5	7.5	25.3	1	1	0
DR-2Mpy/4Mpy		1.029	1.04	1.08	1.03	0.03	0.10	0.01	0.15	0.15	0.14	3.0	9.3	0.8	1	1	1
DR-1Mpy/4Mpy		0.883	0.90	0.91	0.90	0.03	0.05	0.03	0.13	0.13	0.13	3.4	5.8	3.3	1	1	1
DR-SES1/SES2	**m/z123**	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0
DR-SES3/SES5		0.000	0.00	0.19	0.17	0.00	0.37	0.33	0.00	0.03	0.02	NaN	200.0	200.0	0	0	0
DR-SES4/SES6		0.807	0.40	0.91	0.82	0.81	0.20	0.02	0.06	0.13	0.11	200.0	22.5	3.0	0	0	1
DR-SES5/SES10		0.702	0.35	0.93	0.72	0.70	0.46	0.03	0.05	0.13	0.10	200.0	49.7	3.8	0	0	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	**Test Date**	**Sample Description**
1. 2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.8: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0500) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0501 Test Date: 03-Sep-2009 Description: Arendal kommune:Oil with soil and sand

Ratio Name	Spill	Mean			Absolute Difference			Critical Difference			Percentage Difference			Flag*		
		R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3
DR-C28 **m/z191**	0.087	0.04	0.09	0.09	0.09	0.00	0.01	0.01	0.01	0.01	200.0	4.3	5.8	0	1	1
DR-C29	0.099	0.05	0.09	0.10	0.10	0.01	0.01	0.01	0.01	0.01	200.0	14.0	5.8	0	1	1
DR-C28C29	0.186	0.09	0.18	0.19	0.19	0.01	0.00	0.01	0.03	0.03	200.0	5.0	0.2	0	1	1
DR-27Ts	0.491	0.49	0.42	0.51	0.01	0.15	0.03	0.07	0.06	0.07	1.6	35.0	5.9	1	0	1
DR-28ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-25nor30ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-29Ts	0.151	0.14	0.13	0.15	0.02	0.03	0.00	0.02	0.02	0.02	12.2	24.5	0.3	1	0	1
DR-30O	0.043	0.05	0.08	0.04	0.01	0.07	0.01	0.01	0.01	0.01	14.1	92.4	34.1	0	0	0
DR-30G	0.088	0.04	0.04	0.09	0.09	0.09	0.01	0.01	0.01	0.01	200.0	200.0	10.6	0	0	1
DR-29ab	0.737	0.72	0.78	0.73	0.03	0.08	0.01	0.10	0.11	0.10	3.7	10.7	0.8	1	1	1
DR-30d	0.048	0.04	0.04	0.05	0.01	0.01	0.00	0.01	0.01	0.01	17.6	22.5	3.7	0	0	1
DR-29aaS **m/z217**	0.932	0.91	0.89	0.95	0.04	0.09	0.04	0.13	0.12	0.13	4.2	9.7	4.6	1	1	1
DR-29bb **&218**	1.030	NaN	1.05	1.06	NaN	0.04	0.05	NaN	0.15	0.15	NaN	4.2	5.0	0	1	1
DR-27bbSTER	0.514	0.52	0.52	0.51	0.00	0.02	0.01	0.07	0.07	0.07	0.6	3.6	1.2	1	1	1
DR-28bbSTER	0.366	0.37	0.36	0.37	0.01	0.01	0.00	0.05	0.05	0.05	2.9	2.7	0.0	1	1	1
DR-29bbSTER	0.647	0.64	0.64	0.65	0.02	0.01	0.01	0.09	0.09	0.09	2.6	1.2	1.1	1	1	1
DR-TA21 **m/z231**	0.462	0.49	0.63	0.46	0.06	0.34	0.01	0.07	0.09	0.06	13.1	53.5	2.5	1	0	1
DR-TA26	0.440	0.44	0.48	0.46	0.01	0.08	0.04	0.06	0.07	0.06	1.4	16.0	8.1	1	0	1
DR-TA27	0.893	0.90	0.91	0.88	0.02	0.04	0.02	0.13	0.13	0.12	2.6	4.3	2.0	1	1	1
DR-2MP/1MP **PAH**	1.907	2.01	2.05	1.90	0.21	0.29	0.01	0.28	0.29	0.27	10.6	14.2	0.7	1	0	1
DR-4MD/1MD	2.516	2.54	2.63	2.53	0.06	0.23	0.03	0.36	0.37	0.35	2.2	8.8	1.0	1	1	1
DR-C2dbt/C2phe	0.380	0.39	0.37	0.39	0.01	0.02	0.02	0.05	0.05	0.05	3.5	5.5	4.1	1	1	1
DR-C3dbt/C3phe	0.545	0.54	0.52	0.57	0.02	0.04	0.06	0.08	0.07	0.08	3.4	8.3	9.9	1	1	1
DR-C3dbt/C3chr	2.146	2.25	2.17	2.27	0.22	0.04	0.25	0.32	0.30	0.32	9.6	2.0	10.8	1	1	1
DR-Retene/C4phe	0.024	0.01	0.04	0.02	0.02	0.04	0.00	0.00	0.01	0.00	200.0	93.5	4.5	0	0	1
DR-BaF/4Mpy	0.402	0.40	0.36	0.43	0.01	0.08	0.06	0.06	0.05	0.06	2.1	21.1	13.7	1	0	1
DR-BbcF/4Mpy	0.191	0.20	0.18	0.22	0.01	0.02	0.05	0.03	0.03	0.03	4.6	8.5	24.3	1	1	0
DR-2Mpy/4Mpy	1.040	1.05	1.09	1.03	0.02	0.09	0.02	0.15	0.15	0.14	1.9	8.2	1.9	1	1	1
DR-1Mpy/4Mpy	0.892	0.90	0.91	0.90	0.02	0.04	0.02	0.13	0.13	0.13	2.4	4.8	2.3	1	1	1
DR-SES1/SES2 **m/z123**	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0
DR-SES3/SES5	0.000	0.00	0.19	0.17	0.00	0.37	0.33	0.00	0.03	0.02	NaN	200.0	200.0	0	0	0
DR-SES4/SES6	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0
DR-SES5/SES10	0.465	0.23	0.82	0.60	0.47	0.70	0.26	0.03	0.11	0.08	200.0	85.9	44.2	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.9: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0501) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0579 Test Date: Aug-2009 Description: Oil samples from Såstein, respectively 3, 5 and 10 days after casualty

Ratio Name		Spill	Mean			Absolute Difference			Critical Difference			Percentage Difference			Flag*		
			R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3
DR-C28	**m/z191**	0.000	0.00	0.05	0.05	0.00	0.09	0.09	0.00	0.01	0.01	NaN	200.0	200.0	0	0	0
DR-C29		0.000	0.00	0.04	0.05	0.00	0.09	0.09	0.00	0.01	0.01	NaN	200.0	200.0	0	0	0
DR-C28C29		0.000	0.00	0.09	0.09	0.00	0.18	0.19	0.00	0.01	0.01	NaN	200.0	200.0	0	0	0
DR-27Ts		0.483	0.48	0.41	0.50	0.00	0.14	0.04	0.07	0.06	0.07	0.0	33.5	7.5	1	0	1
DR-28ab		0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-25nor30ab		0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-29Ts		0.133	0.13	0.13	0.14	0.00	0.02	0.02	0.02	0.02	0.02	0.0	12.3	11.9	1	1	1
DR-30O		0.050	0.05	0.08	0.04	0.00	0.07	0.02	0.01	0.01	0.01	0.0	80.9	47.6	1	0	0
DR-30G		0.000	0.00	0.00	0.05	0.00	0.00	0.10	0.00	0.00	0.01	NaN	NaN	200.0	0	0	0
DR-29ab		0.710	0.71	0.76	0.72	0.00	0.11	0.02	0.10	0.11	0.10	0.0	14.3	2.9	1	0	1
DR-30d		0.040	0.04	0.04	0.04	0.00	0.00	0.01	0.01	0.01	0.01	0.0	4.9	21.2	1	1	0
DR-29aaS	**m/z217**	0.893	0.89	0.87	0.93	0.00	0.05	0.08	0.13	0.12	0.13	0.0	5.5	8.7	1	1	1
DR-29bb	**&218**	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0
DR-27bbSTER		0.517	0.52	0.52	0.51	0.00	0.02	0.01	0.07	0.07	0.07	0.0	3.1	1.7	1	1	1
DR-28bbSTER		0.377	0.38	0.37	0.37	0.00	0.02	0.01	0.05	0.05	0.05	0.0	5.6	2.9	1	1	1
DR-29bbSTER		0.630	0.63	0.63	0.64	0.00	0.01	0.02	0.09	0.09	0.09	0.0	1.4	3.7	1	1	1
DR-TA21	**m/z231**	0.527	0.53	0.66	0.49	0.00	0.27	0.08	0.07	0.09	0.07	0.0	41.1	15.6	1	0	0
DR-TA26		0.433	0.43	0.47	0.45	0.00	0.08	0.04	0.06	0.07	0.06	0.0	17.5	9.5	1	0	1
DR-TA27		0.917	0.92	0.92	0.90	0.00	0.02	0.04	0.13	0.13	0.13	0.0	1.7	4.7	1	1	1
DR-2MP/1MP	**PAH**	2.120	2.12	2.16	2.01	0.00	0.08	0.23	0.30	0.30	0.28	0.0	3.6	11.3	1	1	1
DR-4MD/1MD		2.573	2.57	2.66	2.56	0.00	0.17	0.03	0.36	0.37	0.36	0.0	6.5	1.2	1	1	1
DR-C2dbt/C2phe		0.393	0.39	0.38	0.39	0.00	0.03	0.00	0.06	0.05	0.06	0.0	9.0	0.6	1	1	1
DR-C3dbt/C3phe		0.527	0.53	0.51	0.56	0.00	0.02	0.08	0.07	0.07	0.08	0.0	4.9	13.3	1	1	1
DR-C3dbt/C3chr		2.363	2.36	2.28	2.38	0.00	0.17	0.03	0.33	0.32	0.33	0.0	7.6	1.2	1	1	1
DR-Retene/C4phe		0.000	0.00	0.03	0.01	0.00	0.07	0.02	0.00	0.00	0.00	NaN	200.0	200.0	0	0	0
DR-BaF/4Mpy		0.393	0.39	0.36	0.43	0.00	0.07	0.07	0.06	0.05	0.06	0.0	19.1	15.7	1	0	0
DR-BbcF/4Mpy		0.200	0.20	0.19	0.22	0.00	0.02	0.04	0.03	0.03	0.03	0.0	13.1	19.8	1	1	0
DR-2Mpy/4Mpy		1.060	1.06	1.09	1.04	0.00	0.07	0.04	0.15	0.15	0.15	0.0	6.4	3.7	1	1	1
DR-1Mpy/4Mpy		0.913	0.91	0.92	0.91	0.00	0.02	0.00	0.13	0.13	0.13	0.0	2.4	0.1	1	1	1
DR-SES1/SES3	**m/z123**	0.000	0.00	1.01	1.16	0.00	2.01	2.31	0.00	0.14	0.16	NaN	200.0	200.0	0	0	0
DR-SES3/SES5		0.000	0.00	0.19	0.17	0.00	0.37	0.33	0.00	0.03	0.02	NaN	200.0	200.0	0	0	0
DR-SES4/SES6		0.000	0.00	0.51	0.42	0.00	1.01	0.83	0.00	0.07	0.06	NaN	200.0	200.0	0	0	0
DR-SES5/SES10		0.000	0.00	0.58	0.36	0.00	1.17	0.73	0.00	0.08	0.05	NaN	200.0	200.0	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.10: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0579) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0602 Test Date: 03-Sep-2009 Description: Cargo no 2:Sample no 1 (Oil from"FullCity")

Ratio Name	**Spill**	**Mean**			**Absolute Difference**			**Critical Difference**			**Percentage Difference**			**Flag***		
		R1	**R2**	**R3**	**R1**	**R2**	**R3**	**R1**	**R2**	**R3**	**R1**	**R2**	**R3**	**R1**	**R2**	**R3**
DR-C28 **m/z191**	0.088	0.04	0.09	0.09	0.09	0.00	0.00	0.01	0.01	0.01	200.0	3.3	4.8	0	1	1
DR-C29	0.096	0.05	0.09	0.09	0.10	0.01	0.00	0.01	0.01	0.01	200.0	11.6	3.4	0	1	1
DR-C28C29	0.185	0.09	0.18	0.19	0.18	0.01	0.00	0.01	0.03	0.03	200.0	4.2	0.6	0	1	1
DR-27Ts	0.613	0.55	0.48	0.57	0.13	0.27	0.09	0.08	0.07	0.08	23.6	56.0	16.2	0	0	0
DR-28ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-25nor30ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-29Ts	0.155	0.14	0.14	0.15	0.02	0.04	0.00	0.02	0.02	0.02	15.1	27.2	3.2	0	0	1
DR-30O	0.000	0.02	0.06	0.02	0.05	0.12	0.03	0.00	0.01	0.00	200.0	200.0	200.0	0	0	0
DR-30G	0.000	0.00	0.00	0.05	0.00	0.00	0.10	0.00	0.00	0.01	NaN	NaN	200.0	0	0	0
DR-29ab	0.727	0.72	0.77	0.73	0.02	0.09	0.00	0.10	0.11	0.10	2.3	12.0	0.5	1	1	1
DR-30d	0.054	0.05	0.05	0.05	0.01	0.02	0.00	0.01	0.01	0.01	29.0	33.8	7.9	0	0	1
DR-29aaS **m/z217**	0.973	0.93	0.91	0.97	0.08	0.13	0.00	0.13	0.13	0.14	8.5	14.0	0.2	1	1	1
DR-29bb **&218**	1.125	NaN	1.10	1.10	NaN	0.05	0.04	NaN	0.15	0.15	NaN	4.7	3.8	0	1	1
DR-27bbSTER	0.501	0.51	0.52	0.50	0.02	0.03	0.01	0.07	0.07	0.07	3.1	6.2	1.4	1	1	1
DR-28bbSTER	0.389	0.38	0.37	0.38	0.01	0.03	0.02	0.05	0.05	0.05	3.2	8.8	6.1	1	1	1
DR-29bbSTER	0.630	0.63	0.63	0.64	0.00	0.01	0.02	0.09	0.09	0.09	0.1	1.4	3.8	1	1	1
DR-TA21 **m/z231**	0.413	0.47	0.61	0.43	0.11	0.39	0.04	0.07	0.08	0.06	24.1	63.6	8.6	0	0	1
DR-TA26	0.440	0.44	0.48	0.46	0.01	0.08	0.04	0.06	0.07	0.06	1.6	15.9	7.9	1	0	1
DR-TA27	0.875	0.90	0.90	0.88	0.04	0.06	0.00	0.13	0.13	0.12	4.6	6.3	0.1	1	1	1
DR-2MP/1MP **PAH**	1.651	1.89	1.92	1.77	0.47	0.55	0.24	0.26	0.27	0.25	24.8	28.4	13.6	0	0	1
DR-4MD/1MD	2.304	2.44	2.53	2.42	0.27	0.44	0.24	0.34	0.35	0.34	11.0	17.6	9.8	1	0	1
DR-C2dbt/C2phe	0.451	0.42	0.41	0.42	0.06	0.09	0.06	0.06	0.06	0.06	13.7	22.6	13.1	1	0	1
DR-C3dbt/C3phe	0.612	0.57	0.56	0.61	0.09	0.11	0.01	0.08	0.08	0.09	15.1	19.9	1.7	0	0	1
DR-C3dbt/C3chr	1.999	2.18	2.09	2.20	0.36	0.19	0.39	0.31	0.29	0.31	16.7	9.1	17.8	0	1	0
DR-Retene/C4phe	0.044	0.02	0.05	0.03	0.04	0.02	0.02	0.00	0.01	0.00	200.0	40.1	54.7	0	0	0
DR-BaF/4Mpy	0.640	0.52	0.48	0.55	0.25	0.32	0.18	0.07	0.07	0.08	47.7	65.3	32.6	0	0	0
DR-BbcF/4Mpy	0.325	0.26	0.25	0.28	0.12	0.15	0.08	0.04	0.04	0.04	47.6	59.7	28.5	0	0	0
DR-2Mpy/4Mpy	0.899	0.98	1.01	0.96	0.16	0.23	0.12	0.14	0.14	0.13	16.5	22.8	12.8	0	0	1
DR-1Mpy/4Mpy	0.887	0.90	0.91	0.90	0.03	0.05	0.03	0.13	0.13	0.13	2.9	5.3	2.8	1	1	1
DR-SES1/SES2 **m/z123**	1.787	0.89	1.90	2.05	1.79	0.22	0.53	0.13	0.27	0.29	200.0	11.7	25.7	0	1	0
DR-SES3/SES5	0.395	0.20	0.38	0.36	0.40	0.02	0.06	0.03	0.05	0.05	200.0	5.5	17.8	0	1	0
DR-SES4/SES6	0.888	0.44	0.95	0.86	0.89	0.12	0.06	0.06	0.13	0.12	200.0	13.0	6.5	0	1	1
DR-SES5/SES10	0.837	0.42	1.00	0.78	0.84	0.33	0.11	0.06	0.14	0.11	200.0	32.9	13.8	0	0	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	**Test Date**	**Sample Description**
1. 2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.11: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0602) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0604 Test Date: 03-Sep-2009 Description: Cargo no 4:Sample no 3 (Oil from"FullCity")

Ratio Name	Spill	Mean			Absolute Difference			Critical Difference			Percentage Difference			Flag*		
		R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3
DR-C28 **m/z191**	0.093	0.05	0.09	0.09	0.09	0.00	0.00	0.01	0.01	0.01	200.0	1.5	0.1	0	1	1
DR-C29	0.093	0.05	0.09	0.09	0.09	0.01	0.00	0.01	0.01	0.01	200.0	8.3	0.1	0	1	1
DR-C28C29	0.186	0.09	0.18	0.19	0.19	0.01	0.00	0.01	0.03	0.03	200.0	4.8	0.0	0	1	1
DR-27Ts	0.562	0.52	0.45	0.54	0.08	0.22	0.04	0.07	0.06	0.08	15.1	48.0	7.6	0	0	1
DR-28ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-25nor30ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-29Ts	0.157	0.15	0.14	0.15	0.02	0.04	0.01	0.02	0.02	0.02	16.6	28.7	4.7	0	0	1
DR-30O	0.000	0.02	0.06	0.02	0.05	0.12	0.03	0.00	0.01	0.00	200.0	200.0	200.0	0	0	0
DR-30G	0.107	0.05	0.05	0.10	0.11	0.11	0.01	0.01	0.01	0.01	200.0	200.0	9.4	0	0	1
DR-29ab	0.743	0.73	0.78	0.74	0.03	0.08	0.01	0.10	0.11	0.10	4.5	9.8	1.6	1	1	1
DR-30d	0.052	0.05	0.04	0.05	0.01	0.01	0.00	0.01	0.01	0.01	25.8	30.6	4.6	0	0	1
DR-29aaS **m/z217**	0.976	0.93	0.91	0.98	0.08	0.13	0.00	0.13	0.13	0.14	8.8	14.3	0.1	1	0	1
DR-29bb **&218**	1.109	NaN	1.09	1.10	NaN	0.04	0.03	NaN	0.15	0.15	NaN	3.2	2.4	0	1	1
DR-27bbSTER	0.484	0.50	0.51	0.50	0.03	0.05	0.02	0.07	0.07	0.07	6.6	9.6	4.8	1	1	1
DR-28bbSTER	0.363	0.37	0.36	0.36	0.01	0.01	0.00	0.05	0.05	0.05	3.6	1.9	0.8	1	1	1
DR-29bbSTER	0.688	0.66	0.66	0.67	0.06	0.05	0.03	0.09	0.09	0.09	8.8	7.4	5.1	1	1	1
DR-TA21 **m/z231**	0.391	0.46	0.60	0.42	0.14	0.41	0.06	0.06	0.08	0.06	29.6	68.6	14.1	0	0	0
DR-TA26	0.428	0.43	0.47	0.45	0.01	0.09	0.05	0.06	0.07	0.06	1.2	18.6	10.7	1	0	1
DR-TA27	0.846	0.88	0.89	0.86	0.07	0.09	0.03	0.12	0.12	0.12	8.0	9.7	3.3	1	1	1
DR-2MP/1MP **PAH**	1.554	1.84	1.88	1.72	0.57	0.64	0.34	0.26	0.26	0.24	30.8	34.3	19.7	0	0	0
DR-4MD/1MD	2.070	2.32	2.41	2.31	0.50	0.68	0.47	0.33	0.34	0.32	21.7	28.1	20.5	0	0	0
DR-C2dbt/C2phe	0.422	0.41	0.39	0.41	0.03	0.06	0.03	0.06	0.05	0.06	7.0	15.9	6.3	1	0	1
DR-C3dbt/C3phe	0.586	0.56	0.54	0.59	0.06	0.08	0.02	0.08	0.08	0.08	10.7	15.6	2.6	1	0	1
DR-C3dbt/C3chr	2.130	2.25	2.16	2.26	0.23	0.06	0.26	0.31	0.30	0.32	10.4	2.8	11.6	1	1	1
DR-Retene/C4phe	0.047	0.02	0.06	0.04	0.05	0.02	0.02	0.00	0.01	0.01	200.0	32.4	62.0	0	0	0
DR-BaF/4Mpy	0.641	0.52	0.48	0.55	0.25	0.32	0.18	0.07	0.07	0.08	47.9	65.5	32.8	0	0	0
DR-BbcF/4Mpy	0.307	0.25	0.24	0.28	0.11	0.13	0.06	0.04	0.03	0.04	42.1	54.4	22.8	0	0	0
DR-2Mpy/4Mpy	0.768	0.91	0.95	0.89	0.29	0.36	0.25	0.13	0.13	0.13	31.9	38.1	28.3	0	0	0
DR-1Mpy/4Mpy	0.837	0.88	0.89	0.87	0.08	0.10	0.08	0.12	0.12	0.12	8.8	11.2	8.6	1	1	1
DR-SES1/SES2 **m/z123**	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	NaN	NaN	NaN	0	0	0
DR-SES3/SES5	0.295	0.15	0.33	0.31	0.29	0.08	0.04	0.02	0.05	0.04	200.0	23.7	11.5	0	0	1
DR-SES4/SES6	0.899	0.45	0.96	0.87	0.90	0.11	0.07	0.06	0.13	0.12	200.0	11.8	7.7	0	1	1
DR-SES5/SES10	1.035	0.52	1.10	0.88	1.03	0.13	0.31	0.07	0.15	0.12	200.0	12.0	34.6	0	1	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.12: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0604) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0606 Test Date: 03-Sep-2009 Description: Machine room:Sample no 5 (Oil from"FullCity")

Ratio Name		Spill	Mean			Absolute Difference			Critical Difference			Percentage Difference			Flag*		
			R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3
DR-C28	**m/z191**	0.046	0.02	0.07	0.07	0.05	0.05	0.05	0.00	0.01	0.01	200.0	65.9	67.2	0	0	0
DR-C29		0.046	0.02	0.07	0.07	0.05	0.04	0.05	0.00	0.01	0.01	200.0	61.2	68.6	0	0	0
DR-C28C29		0.092	0.05	0.13	0.14	0.09	0.09	0.09	0.01	0.02	0.02	200.0	63.6	67.9	0	0	0
DR-27Ts		0.789	0.64	0.57	0.66	0.31	0.44	0.27	0.09	0.08	0.09	48.1	78.4	40.9	0	0	0
DR-28ab		0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-25nor30ab		0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-29Ts		0.181	0.16	0.15	0.17	0.05	0.06	0.03	0.02	0.02	0.02	30.5	42.4	18.8	0	0	0
DR-30O		0.115	0.08	0.12	0.07	0.07	0.00	0.08	0.01	0.02	0.01	78.9	2.4	115.6	0	1	0
DR-30G		0.096	0.05	0.05	0.10	0.10	0.10	0.00	0.01	0.01	0.01	200.0	200.0	1.6	0	0	1
DR-29ab		0.961	0.84	0.89	0.85	0.25	0.14	0.23	0.12	0.12	0.12	30.1	15.9	27.2	0	0	0
DR-30d		0.032	0.04	0.03	0.04	0.01	0.01	0.02	0.01	0.00	0.01	22.8	17.9	43.5	0	0	0
DR-29aaS	**m/z217**	0.870	0.88	0.86	0.92	0.02	0.02	0.10	0.12	0.12	0.13	2.6	2.8	11.4	1	1	1
DR-29bb	**&218**	1.172	NaN	1.12	1.13	NaN	0.10	0.09	NaN	0.16	0.16	NaN	8.7	7.9	0	1	1
DR-27bbSTER		0.384	0.45	0.46	0.45	0.13	0.15	0.12	0.06	0.06	0.06	29.3	32.3	27.6	0	0	0
DR-28bbSTER		0.319	0.35	0.34	0.34	0.06	0.04	0.05	0.05	0.05	0.05	16.6	11.1	13.8	0	1	1
DR-29bbSTER		0.925	0.78	0.78	0.79	0.30	0.29	0.27	0.11	0.11	0.11	38.0	36.6	34.4	0	0	0
DR-TA21	**m/z231**	0.530	0.53	0.66	0.49	0.00	0.27	0.08	0.07	0.09	0.07	0.7	40.4	16.3	1	0	0
DR-TA26		0.415	0.42	0.47	0.45	0.02	0.10	0.06	0.06	0.07	0.06	4.4	21.8	13.9	1	0	1
DR-TA27		0.727	0.82	0.83	0.80	0.19	0.21	0.15	0.12	0.12	0.11	23.1	24.8	18.4	0	0	0
DR-2MP/1MP	**PAH**	1.969	2.04	2.08	1.93	0.15	0.23	0.08	0.29	0.29	0.27	7.4	11.0	3.9	1	1	1
DR-4MD/1MD		3.142	2.86	2.94	2.84	0.57	0.40	0.60	0.40	0.41	0.40	19.9	13.4	21.1	0	1	0
DR-C2dbt/C2phe		0.486	0.44	0.42	0.44	0.09	0.13	0.09	0.06	0.06	0.06	21.2	30.0	20.6	0	0	0
DR-C3dbt/C3phe		0.642	0.58	0.57	0.62	0.12	0.14	0.04	0.08	0.08	0.09	19.8	24.5	6.5	0	0	1
DR-C3dbt/C3chr		2.385	2.37	2.29	2.39	0.02	0.20	0.01	0.33	0.32	0.33	0.9	8.5	0.3	1	1	1
DR-Retene/C4phe		0.034	0.02	0.05	0.03	0.03	0.03	0.01	0.00	0.01	0.00	200.0	62.9	31.4	0	0	0
DR-BaF/4Mpy		0.389	0.39	0.36	0.42	0.00	0.06	0.07	0.05	0.05	0.06	1.2	17.9	16.9	1	0	0
DR-BbcF/4Mpy		0.217	0.21	0.20	0.23	0.02	0.04	0.03	0.03	0.03	0.03	8.1	21.1	11.8	1	0	1
DR-2Mpy/4Mpy		1.184	1.12	1.16	1.10	0.12	0.05	0.16	0.16	0.16	0.15	11.0	4.7	14.8	1	1	0
DR-1Mpy/4Mpy		0.964	0.94	0.95	0.94	0.05	0.03	0.05	0.13	0.13	0.13	5.4	3.0	5.5	1	1	1
DR-SES1/SES2	**m/z123**	1.639	0.82	1.82	1.98	1.64	0.37	0.67	0.11	0.26	0.28	200.0	20.3	34.1	0	0	0
DR-SES3/SES5		0.775	0.39	0.57	0.55	0.78	0.40	0.44	0.05	0.08	0.08	200.0	69.8	80.4	0	0	0
DR-SES4/SES6		1.101	0.55	1.06	0.97	1.10	0.09	0.27	0.08	0.15	0.14	200.0	8.4	27.8	0	1	0
DR-SES5/SES10		0.716	0.36	0.94	0.72	0.72	0.45	0.01	0.05	0.13	0.10	200.0	47.9	1.9	0	0	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.13: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0606) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0609 Test Date: 03-Sep-2009 Description: Vysotsk, Damanskiy:IF180 (sealing No. 9487431)

Ratio Name	Spill	Mean			Absolute Difference			Critical Difference			Percentage Difference			Flag*		
		R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3
DR-C28 **m/z191**	0.066	0.03	0.08	0.08	0.07	0.02	0.03	0.00	0.01	0.01	200.0	31.4	32.9	0	0	0
DR-C29	0.071	0.04	0.08	0.08	0.07	0.01	0.02	0.00	0.01	0.01	200.0	18.5	26.6	0	0	0
DR-C28C29	0.138	0.07	0.16	0.16	0.14	0.04	0.05	0.01	0.02	0.02	200.0	25.0	29.7	0	0	0
DR-27Ts	0.709	0.60	0.53	0.61	0.23	0.36	0.19	0.08	0.07	0.09	37.8	69.1	30.5	0	0	0
DR-28ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-25nor30ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-29Ts	0.160	0.15	0.14	0.15	0.03	0.04	0.01	0.02	0.02	0.02	17.9	30.1	6.0	0	0	1
DR-30O	0.000	0.02	0.06	0.02	0.05	0.12	0.03	0.00	0.01	0.00	200.0	200.0	200.0	0	0	0
DR-30G	0.121	0.06	0.06	0.11	0.12	0.12	0.02	0.01	0.01	0.02	200.0	200.0	21.6	0	0	0
DR-29ab	0.683	0.70	0.75	0.71	0.03	0.14	0.05	0.10	0.11	0.10	3.8	18.2	6.7	1	0	1
DR-30d	0.061	0.05	0.05	0.06	0.02	0.02	0.01	0.01	0.01	0.01	41.0	45.8	20.3	0	0	0
DR-29aaS **m/z217**	1.010	0.95	0.93	0.99	0.12	0.16	0.03	0.13	0.13	0.14	12.2	17.7	3.5	1	0	1
DR-29bb **&218**	1.145	NaN	1.11	1.11	NaN	0.07	0.06	NaN	0.16	0.16	NaN	6.4	5.6	0	1	1
DR-27bbSTER	0.394	0.46	0.46	0.45	0.12	0.14	0.11	0.06	0.06	0.06	27.0	30.0	25.3	0	0	0
DR-28bbSTER	0.329	0.35	0.34	0.35	0.05	0.03	0.04	0.05	0.05	0.05	13.6	8.0	10.7	1	1	1
DR-29bbSTER	0.887	0.76	0.76	0.77	0.26	0.25	0.23	0.11	0.11	0.11	33.9	32.5	30.3	0	0	0
DR-TA21 **m/z231**	0.223	0.37	0.51	0.34	0.30	0.58	0.23	0.05	0.07	0.05	81.1	112.8	67.7	0	0	0
DR-TA26	0.246	0.34	0.38	0.36	0.19	0.27	0.23	0.05	0.05	0.05	55.2	71.0	63.9	0	0	0
DR-TA27	0.441	0.68	0.69	0.66	0.48	0.49	0.43	0.10	0.10	0.09	70.1	71.6	65.9	0	0	0
DR-2MP/1MP **PAH**	1.634	1.88	1.92	1.76	0.49	0.56	0.26	0.26	0.27	0.25	25.9	29.4	14.7	0	0	0
DR-4MD/1MD	2.935	2.75	2.84	2.74	0.36	0.19	0.39	0.39	0.40	0.38	13.1	6.6	14.3	1	1	0
DR-C2dbt/C2phe	0.327	0.36	0.34	0.36	0.07	0.03	0.07	0.05	0.05	0.05	18.6	9.6	19.2	0	1	0
DR-C3dbt/C3phe	0.400	0.46	0.45	0.50	0.13	0.10	0.20	0.06	0.06	0.07	27.3	22.5	40.3	0	0	0
DR-C3dbt/C3chr	1.392	1.88	1.79	1.89	0.97	0.80	1.00	0.26	0.25	0.26	51.7	44.6	52.8	0	0	0
DR-Retene/C4phe	0.049	0.02	0.06	0.04	0.05	0.02	0.02	0.00	0.01	0.01	200.0	27.9	66.2	0	0	0
DR-BaF/4Mpy	0.820	0.61	0.57	0.64	0.43	0.50	0.36	0.08	0.08	0.09	70.4	86.5	56.2	0	0	0
DR-BbcF/4Mpy	0.387	0.29	0.28	0.32	0.19	0.21	0.14	0.04	0.04	0.04	63.7	75.2	45.3	0	0	0
DR-2Mpy/4Mpy	0.902	0.98	1.02	0.96	0.16	0.23	0.12	0.14	0.14	0.13	16.1	22.4	12.4	0	0	1
DR-1Mpy/4Mpy	0.895	0.90	0.92	0.90	0.02	0.04	0.02	0.13	0.13	0.13	2.1	4.5	2.0	1	1	1
DR-SES1/SES8 **m/z123**	0.297	0.15	1.15	1.31	0.30	1.71	2.02	0.02	0.16	0.18	200.0	148.4	154.4	0	0	0
DR-SES3/SES5	0.411	0.21	0.39	0.37	0.41	0.04	0.08	0.03	0.05	0.05	200.0	9.5	21.7	0	1	0
DR-SES4/SES6	0.998	0.50	1.01	0.92	1.00	0.01	0.17	0.07	0.14	0.13	200.0	1.4	18.1	0	1	0
DR-SES5/SES10	0.717	0.36	0.94	0.72	0.72	0.45	0.01	0.05	0.13	0.10	200.0	47.8	1.7	0	0	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.14: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0609) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting — Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0614 Test Date: 03-Sep-2009 Description: Skagen Roads:LS180 (sealing No. 0027014)

Ratio Name	Spill	Mean			Absolute Difference			Critical Difference			Percentage Difference			Flag*		
		R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3
DR-C28 **m/z191**	0.109	0.05	0.10	0.10	0.11	0.02	0.02	0.01	0.01	0.01	200.0	17.7	16.2	0	0	0
DR-C29	0.090	0.05	0.09	0.09	0.09	0.00	0.00	0.01	0.01	0.01	200.0	5.0	3.2	0	1	1
DR-C28C29	0.199	0.10	0.19	0.19	0.20	0.02	0.01	0.01	0.03	0.03	200.0	11.8	6.9	0	1	1
DR-27Ts	0.543	0.51	0.44	0.53	0.06	0.20	0.02	0.07	0.06	0.07	11.6	44.6	4.1	1	0	1
DR-28ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-25nor30ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-29Ts	0.167	0.15	0.14	0.16	0.03	0.05	0.02	0.02	0.02	0.02	22.6	34.7	10.8	0	0	1
DR-30O	0.091	0.07	0.10	0.06	0.04	0.03	0.06	0.01	0.01	0.01	57.9	26.1	98.7	0	0	0
DR-30G	0.078	0.04	0.04	0.09	0.08	0.08	0.02	0.01	0.01	0.01	200.0	200.0	22.4	0	0	0
DR-29ab	0.580	0.65	0.70	0.66	0.13	0.24	0.15	0.09	0.10	0.09	20.1	34.2	22.9	0	0	0
DR-30d	0.090	0.06	0.06	0.07	0.05	0.05	0.04	0.01	0.01	0.01	76.7	80.8	57.8	0	0	0
DR-29aaS **m/z217**	0.739	0.82	0.79	0.86	0.15	0.11	0.24	0.11	0.11	0.12	18.9	13.5	27.5	0	1	0
DR-29bb **&218**	0.829	NaN	0.95	0.96	NaN	0.24	0.25	NaN	0.13	0.13	NaN	25.7	26.5	0	0	0
DR-27bbSTER	0.569	0.54	0.55	0.54	0.05	0.04	0.06	0.08	0.08	0.08	9.7	6.6	11.4	1	1	1
DR-28bbSTER	0.402	0.39	0.38	0.38	0.03	0.05	0.04	0.05	0.05	0.05	6.6	12.2	9.5	1	1	1
DR-29bbSTER	0.539	0.58	0.59	0.60	0.09	0.10	0.11	0.08	0.08	0.08	15.5	16.9	19.2	0	0	0
DR-TA21 **m/z231**	1.711	1.12	1.25	1.08	1.18	0.91	1.26	0.16	0.18	0.15	105.8	72.6	116.6	0	0	0
DR-TA26	0.583	0.51	0.55	0.53	0.15	0.07	0.11	0.07	0.08	0.07	29.4	12.1	20.0	0	1	0
DR-TA27	0.889	0.90	0.91	0.88	0.03	0.04	0.01	0.13	0.13	0.12	3.0	4.7	1.7	1	1	1
DR-2MP/1MP **PAH**	1.848	1.98	2.02	1.87	0.27	0.35	0.05	0.28	0.28	0.26	13.7	17.3	2.4	1	0	1
DR-4MD/1MD	2.934	2.75	2.84	2.74	0.36	0.19	0.39	0.39	0.40	0.38	13.1	6.6	14.3	1	1	0
DR-C2dbt/C2phe	0.268	0.33	0.31	0.33	0.12	0.09	0.13	0.05	0.04	0.05	37.8	29.0	38.4	0	0	0
DR-C3dbt/C3phe	0.336	0.43	0.42	0.47	0.19	0.17	0.27	0.06	0.06	0.07	44.2	39.6	56.7	0	0	0
DR-C3dbt/C3chr	0.842	1.60	1.52	1.62	1.52	1.35	1.55	0.22	0.21	0.23	94.9	88.9	95.8	0	0	0
DR-Retene/C4phe	0.035	0.02	0.05	0.03	0.04	0.03	0.01	0.00	0.01	0.00	200.0	59.3	35.3	0	0	0
DR-BaF/4Mpy	0.524	0.46	0.42	0.49	0.13	0.20	0.06	0.06	0.06	0.07	28.4	46.9	12.8	0	0	1
DR-BbcF/4Mpy	0.283	0.24	0.23	0.26	0.08	0.11	0.04	0.03	0.03	0.04	34.5	47.0	15.0	0	0	0
DR-2Mpy/4Mpy	0.959	1.01	1.04	0.99	0.10	0.17	0.06	0.14	0.15	0.14	10.0	16.3	6.3	1	0	1
DR-1Mpy/4Mpy	0.888	0.90	0.91	0.90	0.03	0.05	0.02	0.13	0.13	0.13	2.8	5.2	2.7	1	1	1
DR-SES1/SES2 **m/z123**	1.370	0.68	1.69	1.84	1.37	0.64	0.94	0.10	0.24	0.26	200.0	37.9	51.3	0	0	0
DR-SES3/SES5	0.315	0.16	0.34	0.32	0.31	0.06	0.02	0.02	0.05	0.05	200.0	17.2	4.9	0	0	1
DR-SES4/SES6	0.788	0.39	0.90	0.81	0.79	0.22	0.04	0.06	0.13	0.11	200.0	24.9	5.5	0	0	1
DR-SES5/SES10	1.495	0.75	1.33	1.11	1.50	0.33	0.77	0.10	0.19	0.16	200.0	24.7	68.9	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.15: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0614) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0616 Test Date: 03-Sep-2009 Description: Skagen Roads:HS180 (sealing No.0027074)

Ratio Name		Spill	Mean			Absolute Difference			Critical Difference			Percentage Difference			Flag*		
			R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3
DR-C28	m/z191	0.138	0.07	0.11	0.12	0.14	0.05	0.05	0.01	0.02	0.02	200.0	40.8	39.3	0	0	0
DR-C29		0.113	0.06	0.10	0.10	0.11	0.03	0.02	0.01	0.01	0.01	200.0	27.6	19.5	0	0	0
DR-C28C29		0.251	0.13	0.21	0.22	0.25	0.07	0.07	0.02	0.03	0.03	200.0	34.7	30.0	0	0	0
DR-27Ts		0.189	0.34	0.27	0.36	0.29	0.16	0.33	0.05	0.04	0.05	87.4	58.2	93.4	0	0	0
DR-28ab		0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-25nor30ab		0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-29Ts		0.096	0.11	0.11	0.12	0.04	0.02	0.05	0.02	0.01	0.02	32.9	20.8	44.4	0	0	0
DR-30O		0.000	0.02	0.06	0.02	0.05	0.12	0.03	0.00	0.01	0.00	200.0	200.0	200.0	0	0	0
DR-30G		0.067	0.03	0.03	0.08	0.07	0.07	0.03	0.00	0.00	0.01	200.0	200.0	37.6	0	0	0
DR-29ab		0.741	0.73	0.78	0.74	0.03	0.08	0.01	0.10	0.11	0.10	4.3	10.0	1.4	1	1	1
DR-30d		0.038	0.04	0.04	0.04	0.00	0.00	0.01	0.01	0.01	0.01	5.4	0.5	26.5	1	1	0
DR-29aaS	m/z217	0.927	0.91	0.89	0.95	0.03	0.08	0.05	0.13	0.12	0.13	3.7	9.2	5.0	1	1	1
DR-29bb	&218	0.917	NaN	1.00	1.00	NaN	0.16	0.17	NaN	0.14	0.14	NaN	15.8	16.7	0	0	0
DR-27bbSTER		0.649	0.58	0.59	0.58	0.13	0.12	0.14	0.08	0.08	0.08	22.7	19.6	24.4	0	0	0
DR-28bbSTER		0.378	0.38	0.37	0.37	0.00	0.02	0.01	0.05	0.05	0.05	0.3	5.9	3.1	1	1	1
DR-29bbSTER		0.498	0.56	0.57	0.58	0.13	0.14	0.16	0.08	0.08	0.08	23.4	24.8	27.1	0	0	0
DR-TA21	m/z231	1.285	0.91	1.04	0.87	0.76	0.49	0.83	0.13	0.15	0.12	83.7	46.6	96.1	0	0	0
DR-TA26		0.613	0.52	0.56	0.54	0.18	0.10	0.14	0.07	0.08	0.08	34.3	17.1	25.0	0	0	0
DR-TA27		1.021	0.97	0.98	0.95	0.10	0.09	0.15	0.14	0.14	0.13	10.8	9.0	15.4	1	1	0
DR-2MP/1MP	PAH	1.943	2.03	2.07	1.92	0.18	0.26	0.05	0.28	0.29	0.27	8.7	12.3	2.6	1	1	1
DR-4MD/1MD		2.255	2.41	2.50	2.40	0.32	0.49	0.29	0.34	0.35	0.34	13.2	19.7	12.0	1	0	1
DR-C2dbt/C2phe		0.257	0.33	0.31	0.33	0.14	0.10	0.14	0.05	0.04	0.05	41.9	33.2	42.5	0	0	0
DR-C3dbt/C3phe		0.399	0.46	0.45	0.50	0.13	0.10	0.20	0.06	0.06	0.07	27.5	22.7	40.4	0	0	0
DR-C3dbt/C3chr		2.196	2.28	2.19	2.29	0.17	0.01	0.20	0.32	0.31	0.32	7.3	0.3	8.5	1	1	1
DR-Retene/C4phe		0.021	0.01	0.04	0.02	0.02	0.04	0.00	0.00	0.01	0.00	200.0	104.0	18.4	0	0	0
DR-BaF/4Mpy		0.273	0.33	0.30	0.37	0.12	0.05	0.19	0.05	0.04	0.05	36.1	17.3	51.1	0	0	0
DR-BbcF/4Mpy		0.150	0.18	0.16	0.20	0.05	0.03	0.09	0.02	0.02	0.03	28.4	15.5	47.5	0	0	0
DR-2Mpy/4Mpy		0.906	0.98	1.02	0.96	0.15	0.22	0.12	0.14	0.14	0.13	15.7	22.0	12.0	0	0	1
DR-1Mpy/4Mpy		0.846	0.88	0.89	0.88	0.07	0.09	0.07	0.12	0.12	0.12	7.7	10.1	7.5	1	1	1
DR-SES1/SES8	m/z123	3.514	1.76	2.76	2.91	3.51	1.50	1.20	0.25	0.39	0.41	200.0	54.4	41.2	0	0	0
DR-SES3/SES5		0.241	0.12	0.31	0.29	0.24	0.13	0.09	0.02	0.04	0.04	200.0	43.3	31.5	0	0	0
DR-SES4/SES6		0.821	0.41	0.92	0.83	0.82	0.19	0.01	0.06	0.13	0.12	200.0	20.9	1.4	0	0	1
DR-SES5/SES10		1.366	0.68	1.27	1.05	1.37	0.20	0.64	0.10	0.18	0.15	200.0	15.7	60.8	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	**Test Date**	**Sample Description**
1. 2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.16: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0616) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0622 Test Date: 03-Sep-2009 Description: Lyngholm, Lillesand:

Ratio Name	Spill	Mean			Absolute Difference			Critical Difference			Percentage Difference			Flag*		
		R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3
DR-C28 **m/z191**	0.088	0.04	0.09	0.09	0.09	0.00	0.01	0.01	0.01	0.01	200.0	4.2	5.7	0	1	1
DR-C29	0.088	0.04	0.09	0.09	0.09	0.00	0.00	0.01	0.01	0.01	200.0	2.7	5.5	0	1	1
DR-C28C29	0.176	0.09	0.18	0.18	0.18	0.00	0.01	0.01	0.02	0.03	200.0	0.8	5.6	0	1	1
DR-27Ts	0.476	0.48	0.41	0.50	0.01	0.13	0.04	0.07	0.06	0.07	1.5	32.0	9.0	1	0	1
DR-28ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-25nor30ab	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	NaN	NaN	NaN	0	0	0
DR-29Ts	0.152	0.14	0.14	0.15	0.02	0.03	0.00	0.02	0.02	0.02	13.3	25.5	1.4	1	0	1
DR-30O	0.047	0.05	0.08	0.04	0.00	0.07	0.02	0.01	0.01	0.01	6.4	86.2	41.5	1	0	0
DR-30G	0.093	0.05	0.05	0.10	0.09	0.09	0.00	0.01	0.01	0.01	200.0	200.0	4.3	0	0	1
DR-29ab	0.742	0.73	0.78	0.74	0.03	0.08	0.01	0.10	0.11	0.10	4.4	10.0	1.5	1	1	1
DR-30d	0.048	0.04	0.04	0.05	0.01	0.01	0.00	0.01	0.01	0.01	18.6	23.5	2.6	0	0	1
DR-29aaS **m/z217**	0.920	0.91	0.88	0.95	0.03	0.07	0.05	0.13	0.12	0.13	3.0	8.4	5.8	1	1	1
DR-29bb **&218**	1.026	NaN	1.05	1.05	NaN	0.05	0.06	NaN	0.15	0.15	NaN	4.6	5.4	0	1	1
DR-27bbSTER	0.512	0.51	0.52	0.51	0.00	0.02	0.00	0.07	0.07	0.07	0.9	3.9	0.9	1	1	1
DR-28bbSTER	0.372	0.37	0.36	0.37	0.00	0.02	0.01	0.05	0.05	0.05	1.2	4.3	1.6	1	1	1
DR-29bbSTER	0.640	0.63	0.64	0.65	0.01	0.00	0.01	0.09	0.09	0.09	1.5	0.2	2.1	1	1	1
DR-TA21 **m/z231**	0.479	0.50	0.64	0.46	0.05	0.32	0.03	0.07	0.09	0.07	9.5	50.2	6.1	1	0	1
DR-TA26	0.444	0.44	0.48	0.46	0.01	0.07	0.03	0.06	0.07	0.06	2.5	15.0	7.0	1	0	1
DR-TA27	0.874	0.90	0.90	0.87	0.04	0.06	0.00	0.13	0.13	0.12	4.7	6.5	0.1	1	1	1
DR-2MP/1MP **PAH**	1.948	2.03	2.07	1.92	0.17	0.25	0.05	0.28	0.29	0.27	8.5	12.1	2.9	1	1	1
DR-4MD/1MD	2.477	2.52	2.61	2.51	0.10	0.27	0.07	0.35	0.37	0.35	3.8	10.4	2.6	1	1	1
DR-C2dbt/C2phe	0.432	0.41	0.40	0.41	0.04	0.07	0.04	0.06	0.06	0.06	9.4	18.3	8.8	1	0	1
DR-C3dbt/C3phe	0.560	0.54	0.53	0.58	0.03	0.06	0.04	0.08	0.07	0.08	6.1	10.9	7.2	1	1	1
DR-C3dbt/C3chr	2.382	2.37	2.29	2.39	0.02	0.19	0.01	0.33	0.32	0.33	0.8	8.4	0.4	1	1	1
DR-Retene/C4phe	0.025	0.01	0.05	0.02	0.02	0.04	0.00	0.00	0.01	0.00	200.0	90.1	0.3	0	0	1
DR-BaF/4Mpy	0.416	0.40	0.37	0.44	0.02	0.09	0.04	0.06	0.05	0.06	5.7	24.7	10.1	1	0	1
DR-BbcF/4Mpy	0.203	0.20	0.19	0.22	0.00	0.03	0.04	0.03	0.03	0.03	1.4	14.5	18.4	1	0	0
DR-2Mpy/4Mpy	1.050	1.06	1.09	1.04	0.01	0.08	0.03	0.15	0.15	0.15	0.9	7.3	2.8	1	1	1
DR-1Mpy/4Mpy	0.886	0.90	0.91	0.90	0.03	0.05	0.03	0.13	0.13	0.13	3.0	5.4	2.9	1	1	1
DR-SES1/SES2 **m/z123**	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0
DR-SES3/SES5	0.000	0.00	0.19	0.17	0.00	0.37	0.33	0.00	0.03	0.02	NaN	200.0	200.0	0	0	0
DR-SES4/SES6	0.761	0.38	0.89	0.80	0.76	0.25	0.07	0.05	0.12	0.11	200.0	28.3	8.9	0	0	1
DR-SES5/SES10	0.563	0.28	0.86	0.65	0.56	0.60	0.17	0.04	0.12	0.09	200.0	69.9	25.8	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.17: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0622) and the reference samples.

Evaluation of The Diagnostic Ratio – MV Full City Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2009-0626 Test Date: 09-Oct-2009 Description: No description is available.

Ratio Name	Spill	Mean			Absolute Difference			Critical Difference			Percentage Difference			Flag*		
		R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3	R1	R2	R3
DR-C28 **m/z191**	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0
DR-C29	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0
DR-C28C29	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0
DR-27Ts	0.892	0.69	0.62	0.71	0.41	0.55	0.37	0.10	0.09	0.10	59.5	88.5	52.5	0	0	0
DR-28ab	0.111	0.06	0.06	0.06	0.11	0.11	0.11	0.01	0.01	0.01	200.0	200.0	200.0	0	0	0
DR-25nor30ab	0.081	0.04	0.04	0.04	0.08	0.08	0.08	0.01	0.01	0.01	200.0	200.0	200.0	0	0	0
DR-29Ts	0.212	0.17	0.16	0.18	0.08	0.09	0.06	0.02	0.02	0.03	45.5	57.0	34.1	0	0	0
DR-30O	0.000	0.02	0.06	0.02	0.05	0.12	0.03	0.00	0.01	0.00	200.0	200.0	200.0	0	0	0
DR-30G	0.000	0.00	0.00	0.05	0.00	0.00	0.10	0.00	0.00	0.01	NaN	NaN	200.0	0	0	0
DR-29ab	0.869	0.79	0.84	0.80	0.16	0.05	0.14	0.11	0.12	0.11	20.2	5.9	17.3	0	1	0
DR-30d	0.064	0.05	0.05	0.06	0.02	0.03	0.01	0.01	0.01	0.01	46.6	51.3	26.1	0	0	0
DR-29aaS **m/z217**	1.146	1.02	1.00	1.06	0.25	0.30	0.17	0.14	0.14	0.15	24.8	30.2	16.1	0	0	0
DR-29bb **&218**	1.337	NaN	1.21	1.21	NaN	0.26	0.25	NaN	0.17	0.17	NaN	21.8	21.0	0	0	0
DR-27bbSTER	0.467	0.49	0.50	0.49	0.05	0.07	0.04	0.07	0.07	0.07	10.2	13.2	8.4	1	1	1
DR-28bbSTER	0.404	0.39	0.38	0.39	0.03	0.05	0.04	0.05	0.05	0.05	7.1	12.6	10.0	1	1	1
DR-29bbSTER	0.650	0.64	0.64	0.65	0.02	0.01	0.00	0.09	0.09	0.09	3.1	1.7	0.6	1	1	1
DR-TA21 **m/z231**	0.550	0.54	0.67	0.50	0.02	0.25	0.10	0.08	0.09	0.07	4.3	37.0	19.8	1	0	0
DR-TA26	0.331	0.38	0.42	0.40	0.10	0.19	0.15	0.05	0.06	0.06	26.9	43.9	36.2	0	0	0
DR-TA27	1.016	0.97	0.97	0.95	0.10	0.08	0.14	0.14	0.14	0.13	10.2	8.5	14.9	1	1	0
DR-2MP/1MP **PAH**	1.222	1.67	1.71	1.56	0.90	0.98	0.67	0.23	0.24	0.22	53.7	57.1	43.1	0	0	0
DR-4MD/1MD	2.661	2.62	2.70	2.60	0.09	0.09	0.12	0.37	0.38	0.36	3.4	3.2	4.6	1	1	1
DR-C2dbt/C2phe	0.195	0.29	0.28	0.30	0.20	0.16	0.20	0.04	0.04	0.04	67.2	59.1	67.8	0	0	0
DR-C3dbt/C3phe	0.247	0.39	0.37	0.42	0.28	0.26	0.36	0.05	0.05	0.06	72.4	68.2	83.7	0	0	0
DR-C3dbt/C3chr	1.253	1.81	1.72	1.82	1.11	0.94	1.14	0.25	0.24	0.26	61.4	54.4	62.5	0	0	0
DR-Retene/C4phe	0.403	0.20	0.23	0.21	0.40	0.34	0.38	0.03	0.03	0.03	200.0	144.1	176.8	0	0	0
DR-BaF/4Mpy	1.969	1.18	1.15	1.21	1.58	1.64	1.51	0.17	0.16	0.17	133.4	143.4	124.2	0	0	0
DR-BbcF/4Mpy	0.944	0.57	0.56	0.59	0.74	0.77	0.70	0.08	0.08	0.08	130.1	137.3	117.9	0	0	0
DR-2Mpy/4Mpy	1.114	1.09	1.12	1.07	0.05	0.02	0.09	0.15	0.16	0.15	5.0	1.4	8.7	1	1	1
DR-1Mpy/4Mpy	0.692	0.80	0.81	0.80	0.22	0.24	0.22	0.11	0.11	0.11	27.5	29.9	27.4	0	0	0
DR-SES1/SES2 **m/z123**	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0
DR-SES3/SES5	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0
DR-SES4/SES6	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0
DR-SES5/SES10	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2009-0579	Aug-2009	Oil samples from Såstein, respectively 3, 5 and 10 days after casualty
2. 2009-0485	03-Sep-2009	Krogshavn:20 Liter with smooth, fine emulsion pumped up in krogshavn
3. 2009-0472	03-Sep-2009	Oddane in Vestfold:sand / stones contaminated with oil

Figure D.18: Evaluation of diagnostic ratio (CEN Methods) of "Full City" case (SINTEF ID: 2009-0626) and the reference samples.

E

EVALUATION OF DIAGNOSTIC RATIO (CEN METHODS): "SERVER" CASE

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007-0014 Test Date: 15-Jan-2007 Description: PadSample from sheen/rainbow Oil film outside the lihgthouse at Fedje.

Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR-C28 **m/z191**	0.086	0.15	0.15	0.16	0.16	0.16	0.13	0.12	0.15	0.15	0.14	0.02	0.02	0.02	0.02	0.02	87.6	83.0	94.0	92.4	89.4	0	0	0	0	0
DR-C29	0.084	0.12	0.12	0.13	0.12	0.12	0.08	0.08	0.09	0.08	0.08	0.02	0.02	0.02	0.02	0.02	64.8	64.3	70.1	63.2	65.6	0	0	0	0	0
DR-C28C29	0.170	0.28	0.27	0.29	0.28	0.28	0.21	0.20	0.24	0.23	0.22	0.04	0.04	0.04	0.04	0.04	77.4	74.5	83.4	79.7	78.8	0	0	0	0	0
DR-27Ts	0.647	0.58	0.58	0.59	0.58	0.58	0.13	0.13	0.10	0.14	0.13	0.08	0.08	0.08	0.08	0.08	22.6	23.1	17.4	24.3	21.8	0	0	0	0	0
DR-28ab	0.049	0.10	0.08	0.09	0.09	0.09	0.10	0.07	0.09	0.09	0.09	0.01	0.01	0.01	0.01	0.01	100.8	83.9	95.9	95.3	94.3	0	0	0	0	0
DR-25nor30ab	0.032	0.05	0.04	0.04	0.05	0.05	0.04	0.02	0.03	0.03	0.03	0.01	0.01	0.01	0.01	0.01	72.1	53.3	56.7	65.8	62.4	0	0	0	0	0
DR-29Ts	0.167	0.17	0.16	0.16	0.16	0.16	0.00	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.02	1.7	6.0	7.8	5.7	5.3	1	1	1	1	1
DR-30O	0.119	0.11	0.12	0.10	0.11	0.11	0.03	0.00	0.03	0.02	0.02	0.01	0.02	0.01	0.02	0.02	25.5	3.4	30.7	21.3	19.7	0	1	0	0	0
DR-30G	0.086	0.11	0.10	0.11	0.11	0.11	0.05	0.03	0.05	0.04	0.04	0.02	0.01	0.02	0.01	0.02	47.4	32.0	43.3	38.8	40.6	0	0	0	0	0
DR-29ab	1.045	0.97	0.99	0.96	0.99	0.98	0.14	0.10	0.18	0.12	0.14	0.14	0.14	0.13	0.14	0.14	14.8	10.3	18.5	12.0	13.8	0	1	0	1	1
DR-30d	0.026	0.04	0.03	0.03	0.04	0.04	0.03	0.02	0.02	0.02	0.02	0.01	0.00	0.00	0.00	0.01	69.1	45.2	47.2	50.1	53.5	0	0	0	0	0
DR-29aaS **m/z217**	0.862	0.87	0.88	0.86	0.89	0.87	0.01	0.03	0.00	0.05	0.02	0.12	0.12	0.12	0.12	0.12	1.1	3.2	0.3	6.1	2.7	1	1	1	1	1
DR-29bb **&218**	1.076	1.03	0.99	1.03	1.00	1.01	0.09	0.18	0.09	0.16	0.13	0.14	0.14	0.14	0.14	0.14	9.0	18.3	8.9	15.5	12.8	1	0	1	0	1
DR-27bbSTER	0.501	0.62	0.62	0.63	0.62	0.63	0.25	0.24	0.26	0.24	0.25	0.09	0.09	0.09	0.09	0.09	39.5	38.6	41.6	39.0	39.7	0	0	0	0	0
DR-28bbSTER	0.321	0.31	0.32	0.32	0.32	0.32	0.01	0.01	0.00	0.01	0.01	0.04	0.04	0.04	0.04	0.04	4.5	1.7	1.2	3.2	2.7	1	1	1	1	1
DR-29bbSTER	0.733	0.62	0.62	0.61	0.62	0.62	0.22	0.23	0.25	0.23	0.23	0.09	0.09	0.09	0.09	0.09	36.1	37.3	41.0	36.5	37.7	0	0	0	0	0
DR-TA21 **m/z231**	1.672	3.27	2.82	3.16	3.14	3.09	3.19	2.29	2.97	2.93	2.84	0.46	0.39	0.44	0.44	0.43	97.6	81.2	94.0	93.4	91.9	0	0	0	0	0
DR-TA26	0.394	0.42	0.44	0.42	0.41	0.42	0.05	0.09	0.05	0.04	0.05	0.06	0.06	0.06	0.06	0.06	11.5	20.4	11.1	8.8	13.0	1	0	1	1	1
DR-TA27	1.177	1.10	1.11	1.10	1.10	1.10	0.15	0.13	0.16	0.15	0.15	0.15	0.16	0.15	0.15	0.15	13.3	11.8	14.4	13.8	13.3	1	1	0	1	1
DR-2MP/1MP **PAH**	2.018	2.08	2.10	2.08	2.09	2.09	0.13	0.15	0.13	0.13	0.14	0.29	0.29	0.29	0.29	0.29	6.0	7.4	6.3	6.5	6.5	1	1	1	1	1
DR-4MD/1MD	2.824	2.63	2.64	2.62	2.63	2.63	0.39	0.36	0.41	0.38	0.39	0.37	0.37	0.37	0.37	0.37	14.8	13.7	15.7	14.4	14.7	0	1	0	0	0
DR-C2dbt/C2phe	0.581	0.60	0.62	0.60	0.61	0.61	0.04	0.08	0.03	0.05	0.05	0.08	0.09	0.08	0.08	0.08	7.4	13.5	4.8	8.2	8.5	1	1	1	1	1
DR-C3dbt/C3phe	0.784	0.79	0.81	0.78	0.78	0.79	0.01	0.05	0.02	0.00	0.01	0.11	0.11	0.11	0.11	0.11	1.4	6.2	2.4	0.1	1.4	1	1	1	1	1
DR-C3dbt/C3chr	2.795	2.87	3.08	2.71	2.82	2.87	0.15	0.57	0.18	0.05	0.15	0.40	0.43	0.38	0.39	0.40	5.3	18.5	6.6	1.6	5.1	1	0	1	1	1
DR-Retene/C4phe	0.055	0.05	0.05	0.05	0.05	0.05	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	20.1	21.0	23.5	19.2	21.0	0	0	0	0	0
DR-BaF/4Mpy	0.449	0.46	0.45	0.45	0.45	0.45	0.01	0.01	0.01	0.01	0.01	0.06	0.06	0.06	0.06	0.06	3.0	1.3	1.4	1.8	1.8	1	1	1	1	1
DR-BbcF/4Mpy	0.254	0.27	0.27	0.27	0.27	0.27	0.03	0.03	0.03	0.03	0.03	0.04	0.04	0.04	0.04	0.04	10.4	10.6	9.7	10.8	10.4	1	1	1	1	1
DR-2Mpy/4Mpy	0.903	0.93	0.93	0.93	0.94	0.93	0.05	0.06	0.05	0.07	0.06	0.13	0.13	0.13	0.13	0.13	5.5	6.1	5.6	7.9	6.3	1	1	1	1	1
DR-1Mpy/4Mpy	0.872	0.90	0.90	0.92	0.90	0.91	0.06	0.05	0.10	0.05	0.07	0.13	0.13	0.13	0.13	0.13	6.7	5.5	11.2	6.0	7.4	1	1	1	1	1
DR-SES1/SES2 **m/z123**	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0	0	0
DR-SES3/SES5	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0	0	0
DR-SES4/SES6	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0	0	0
DR-SES5/SES10	0.000	0.45	0.49	0.47	0.47	0.47	0.90	0.98	0.93	0.94	0.94	0.06	0.07	0.07	0.07	0.07	200.0	200.0	200.0	200.0	200.0	0	0	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2007-0017	06-Feb-2007	Emulsion from "TV-bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2. 2007-0023	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 3
3. 2007-0024	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 4
4. 2007-0033	07-Feb-2007	Oil sample collected at KV " Eigun"

Figure E.1: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0014) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007-0024 Test Date: 07-Feb-2007 Description: Oil from shipwreck – "Server": Sample from Tank 4

Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR-C28 **m/z191**	0.239	0.23	0.22	0.24	0.24	0.23	0.02	0.03	0.00	0.01	0.01	0.03	0.03	0.03	0.03	0.03	8.0	13.7	0.0	2.1	5.8	1	1	1	1	1
DR-C29	0.174	0.17	0.17	0.17	0.17	0.17	0.01	0.01	0.00	0.01	0.01	0.02	0.02	0.02	0.02	0.02	5.9	6.5	0.0	7.7	5.0	1	1	1	1	1
DR-C28C29	0.414	0.40	0.39	0.41	0.40	0.40	0.03	0.04	0.00	0.02	0.02	0.06	0.05	0.06	0.06	0.06	7.1	10.6	0.0	4.4	5.5	1	1	1	1	1
DR-27Ts	0.543	0.53	0.53	0.54	0.52	0.53	0.03	0.03	0.00	0.04	0.02	0.07	0.07	0.08	0.07	0.07	5.2	5.8	0.0	6.9	4.4	1	1	1	1	1
DR-28ab	0.138	0.14	0.13	0.14	0.14	0.14	0.01	0.02	0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.02	6.5	15.0	0.0	0.8	2.0	1	0	1	1	1
DR-25nor30ab	0.058	0.06	0.06	0.06	0.06	0.06	0.01	0.00	0.00	0.01	0.00	0.01	0.01	0.01	0.01	0.01	17.1	3.8	0.0	10.0	6.2	0	1	1	1	1
DR-29Ts	0.155	0.16	0.16	0.15	0.16	0.16	0.01	0.00	0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.02	6.1	1.8	0.0	2.1	2.5	1	1	1	1	1
DR-30O	0.087	0.09	0.10	0.09	0.09	0.09	0.00	0.03	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	5.4	27.4	0.0	9.6	11.2	1	0	1	1	1
DR-30G	0.134	0.14	0.13	0.13	0.13	0.13	0.01	0.01	0.00	0.01	0.00	0.02	0.02	0.02	0.02	0.02	4.3	11.7	0.0	4.7	2.9	1	1	1	1	1
DR-29ab	0.868	0.88	0.91	0.87	0.90	0.89	0.03	0.07	0.00	0.06	0.04	0.12	0.13	0.12	0.13	0.12	3.8	8.3	0.0	6.6	4.7	1	1	1	1	1
DR-30d	0.043	0.05	0.04	0.04	0.04	0.04	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	23.9	2.0	0.0	3.1	6.8	0	1	1	1	1
DR-29aaS **m/z217**	0.864	0.87	0.88	0.86	0.89	0.87	0.01	0.03	0.00	0.05	0.02	0.12	0.12	0.12	0.12	0.12	0.8	2.9	0.0	5.8	2.4	1	1	1	1	1
DR-29bb **&218**	0.985	0.98	0.94	0.98	0.95	0.97	0.00	0.09	0.00	0.06	0.04	0.14	0.13	0.14	0.13	0.14	0.2	9.4	0.0	6.7	4.0	1	1	1	1	1
DR-27bbSTER	0.764	0.76	0.75	0.76	0.75	0.76	0.02	0.02	0.00	0.02	0.02	0.11	0.11	0.11	0.11	0.11	2.2	3.1	0.0	2.7	2.0	1	1	1	1	1
DR-28bbSTER	0.317	0.31	0.32	0.32	0.31	0.31	0.01	0.00	0.00	0.01	0.00	0.04	0.04	0.04	0.04	0.04	3.3	0.5	0.0	2.0	1.5	1	1	1	1	1
DR-29bbSTER	0.484	0.50	0.49	0.48	0.50	0.49	0.03	0.02	0.00	0.02	0.02	0.07	0.07	0.07	0.07	0.07	5.1	3.9	0.0	4.7	3.4	1	1	1	1	1
DR-TA21 **m/z231**	4.641	4.75	4.30	4.64	4.62	4.58	0.22	0.68	0.00	0.04	0.13	0.67	0.60	0.65	0.65	0.64	4.7	15.9	0.0	0.9	2.7	1	0	1	1	1
DR-TA26	0.440	0.44	0.46	0.44	0.43	0.44	0.00	0.04	0.00	0.01	0.01	0.06	0.06	0.06	0.06	0.06	0.4	9.3	0.0	2.4	1.9	1	1	1	1	1
DR-TA27	1.019	1.02	1.03	1.02	1.02	1.02	0.01	0.03	0.00	0.01	0.01	0.14	0.14	0.14	0.14	0.14	1.2	2.7	0.0	0.7	1.1	1	1	1	1	1
DR-2MP/1MP **PAH**	2.149	2.15	2.16	2.15	2.15	2.15	0.01	0.02	0.00	0.00	0.01	0.30	0.30	0.30	0.30	0.30	0.2	1.1	0.0	0.2	0.3	1	1	1	1	1
DR-4MD/1MD	2.414	2.42	2.44	2.41	2.43	2.43	0.02	0.05	0.00	0.03	0.02	0.34	0.34	0.34	0.34	0.34	0.9	1.9	0.0	1.3	1.0	1	1	1	1	1
DR-C2dbt/C2phe	0.610	0.62	0.64	0.61	0.62	0.62	0.02	0.06	0.00	0.02	0.02	0.09	0.09	0.09	0.09	0.09	2.6	8.7	0.0	3.5	3.8	1	1	1	1	1
DR-C3dbt/C3phe	0.766	0.78	0.80	0.77	0.78	0.78	0.03	0.07	0.00	0.02	0.03	0.11	0.11	0.11	0.11	0.11	3.8	8.5	0.0	2.5	3.7	1	1	1	1	1
DR-C3dbt/C3chr	2.616	2.78	2.99	2.62	2.73	2.78	0.33	0.75	0.00	0.22	0.33	0.39	0.42	0.37	0.38	0.39	11.9	25.0	0.0	8.2	11.7	1	0	1	1	1
DR-Retene/C4phe	0.043	0.04	0.04	0.04	0.04	0.04	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	3.4	2.5	0.0	4.4	2.6	1	1	1	1	1
DR-BaF/4Mpy	0.455	0.46	0.45	0.46	0.46	0.46	0.01	0.00	0.00	0.00	0.00	0.06	0.06	0.06	0.06	0.06	1.7	0.1	0.0	0.4	0.5	1	1	1	1	1
DR-BbcF/4Mpy	0.280	0.28	0.28	0.28	0.28	0.28	0.00	0.00	0.00	0.00	0.00	0.04	0.04	0.04	0.04	0.04	0.7	0.9	0.0	1.1	0.7	1	1	1	1	1
DR-2Mpy/4Mpy	0.954	0.95	0.96	0.95	0.97	0.96	0.00	0.00	0.00	0.02	0.01	0.13	0.13	0.13	0.14	0.13	0.0	0.5	0.0	2.4	0.7	1	1	1	1	1
DR-1Mpy/4Mpy	0.975	0.95	0.95	0.97	0.95	0.96	0.04	0.05	0.00	0.05	0.04	0.13	0.13	0.14	0.13	0.13	4.5	5.7	0.0	5.2	3.8	1	1	1	1	1
DR-SES1/SES5 **m/z123**	1.723	1.67	1.70	1.72	1.72	1.70	0.10	0.05	0.00	0.01	0.04	0.23	0.24	0.24	0.24	0.24	6.2	2.7	0.0	0.4	2.3	1	1	1	1	1
DR-SES3/SES5	0.403	0.43	0.40	0.40	0.41	0.41	0.05	0.01	0.00	0.01	0.01	0.06	0.06	0.06	0.06	0.06	12.7	3.6	0.0	2.9	3.2	1	1	1	1	1
DR-SES4/SES6	0.915	0.98	0.96	0.92	0.94	0.95	0.13	0.08	0.00	0.04	0.07	0.14	0.13	0.13	0.13	0.13	13.5	8.7	0.0	4.8	6.9	1	1	1	1	1
DR-SES5/SES10	0.933	0.91	0.96	0.93	0.94	0.93	0.04	0.05	0.00	0.01	0.00	0.13	0.13	0.13	0.13	0.13	4.1	5.3	0.0	0.6	0.5	1	1	1	1	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2007-0017	06-Feb-2007	Emulsion from "TV-bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2. 2007-0023	07-Feb-2007	Oil from shipwreck – "Server": Sample from Tank 3
3. 2007-0024	07-Feb-2007	Oil from shipwreck – "Server": Sample from Tank 4
4. 2007-0033	07-Feb-2007	Oil sample collected at KV " Eigun"

Figure E.2: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0024) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007-0068 Test Date: 08-Feb-2007 Description: Bird feathers from dead eiders (nr. 5), Osnessanden, Ulstein

Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR-C28 **m/z191**	0.172	0.20	0.19	0.21	0.20	0.20	0.05	0.04	0.07	0.06	0.05	0.03	0.03	0.03	0.03	0.03	25.0	19.4	32.9	30.8	27.2	0	0	0	0	0
DR-C29	0.141	0.15	0.15	0.16	0.15	0.15	0.02	0.02	0.03	0.02	0.02	0.02	0.02	0.02	0.02	0.02	15.3	14.7	21.1	13.5	16.2	0	0	0	1	0
DR-C28C29	0.313	0.35	0.34	0.36	0.35	0.35	0.07	0.06	0.10	0.08	0.08	0.05	0.05	0.05	0.05	0.05	20.8	17.3	27.8	23.4	22.4	0	0	0	0	0
DR-27Ts	0.541	0.53	0.53	0.54	0.52	0.53	0.03	0.03	0.00	0.03	0.02	0.07	0.07	0.08	0.07	0.07	4.9	5.5	0.3	6.6	4.1	1	1	1	1	1
DR-28ab	0.098	0.12	0.11	0.12	0.12	0.12	0.05	0.02	0.04	0.04	0.04	0.02	0.02	0.02	0.02	0.02	39.9	18.9	33.6	32.9	31.6	0	0	0	0	0
DR-25nor30ab	0.051	0.06	0.05	0.05	0.06	0.06	0.02	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	28.6	7.9	11.6	21.6	17.8	0	1	1	0	0
DR-29Ts	0.154	0.16	0.16	0.15	0.16	0.16	0.01	0.00	0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.02	6.3	2.1	0.3	2.4	2.8	1	1	1	1	1
DR-30O	0.088	0.09	0.10	0.09	0.09	0.09	0.00	0.03	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	4.8	26.9	0.6	9.0	10.6	1	0	1	1	1
DR-30G	0.111	0.13	0.11	0.12	0.12	0.12	0.03	0.01	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	22.8	6.8	18.5	13.8	15.7	0	1	0	1	0
DR-29ab	0.923	0.91	0.93	0.90	0.93	0.92	0.02	0.02	0.05	0.00	0.01	0.13	0.13	0.13	0.13	0.13	2.4	2.1	6.1	0.4	1.4	1	1	1	1	1
DR-30d	0.040	0.05	0.04	0.04	0.04	0.04	0.01	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01	29.3	3.5	5.6	8.7	12.4	0	1	1	1	1
DR-29aaS **m/z217**	0.883	0.88	0.89	0.87	0.90	0.88	0.01	0.01	0.02	0.03	0.00	0.12	0.12	0.12	0.13	0.12	1.4	0.7	2.2	3.7	0.2	1	1	1	1	1
DR-29bb **&218**	1.046	1.01	0.97	1.02	0.98	1.00	0.06	0.15	0.06	0.13	0.10	0.14	0.14	0.14	0.14	0.14	6.2	15.5	6.0	12.7	10.0	1	0	1	1	1
DR-27bbSTER	0.645	0.70	0.69	0.70	0.69	0.70	0.10	0.10	0.12	0.10	0.10	0.10	0.10	0.10	0.10	0.10	14.8	13.9	17.0	14.3	15.0	0	1	0	0	0
DR-28bbSTER	0.326	0.32	0.32	0.32	0.32	0.32	0.02	0.01	0.01	0.02	0.01	0.04	0.04	0.05	0.04	0.04	6.1	3.3	2.8	4.8	4.3	1	1	1	1	1
DR-29bbSTER	0.568	0.54	0.54	0.53	0.54	0.53	0.06	0.06	0.08	0.06	0.07	0.08	0.07	0.07	0.08	0.07	10.9	12.1	16.0	11.3	12.6	1	1	0	1	1
DR-TA21 **m/z231**	2.955	3.91	3.46	3.80	3.78	3.74	1.91	1.00	1.69	1.64	1.56	0.55	0.48	0.53	0.53	0.52	48.8	29.0	44.4	43.5	41.8	0	0	0	0	0
DR-TA26	0.434	0.44	0.46	0.44	0.43	0.44	0.01	0.05	0.01	0.00	0.01	0.06	0.06	0.06	0.06	0.06	1.6	10.6	1.3	1.1	3.2	1	1	1	1	1
DR-TA27	1.045	1.04	1.05	1.03	1.04	1.04	0.01	0.00	0.03	0.02	0.01	0.15	0.15	0.14	0.14	0.15	1.4	0.1	2.6	1.9	1.4	1	1	1	1	1
DR-2MP/1MP **PAH**	2.120	2.13	2.15	2.13	2.14	2.14	0.02	0.05	0.03	0.03	0.03	0.30	0.30	0.30	0.30	0.30	1.1	2.5	1.4	1.6	1.6	1	1	1	1	1
DR-4MD/1MD	2.574	2.50	2.52	2.49	2.51	2.51	0.14	0.11	0.16	0.13	0.14	0.35	0.35	0.35	0.35	0.35	5.6	4.5	6.5	5.2	5.4	1	1	1	1	1
DR-C2dbt/C2phe	0.649	0.64	0.66	0.63	0.64	0.64	0.02	0.02	0.04	0.02	0.02	0.09	0.09	0.09	0.09	0.09	3.7	2.4	6.3	2.9	2.6	1	1	1	1	1
DR-C3dbt/C3phe	0.829	0.81	0.83	0.80	0.81	0.81	0.03	0.00	0.06	0.04	0.03	0.11	0.12	0.11	0.11	0.11	4.2	0.6	8.0	5.5	4.2	1	1	1	1	1
DR-C3dbt/C3chr	3.373	3.16	3.37	2.99	3.11	3.16	0.43	0.01	0.76	0.53	0.43	0.44	0.47	0.42	0.43	0.44	13.5	0.3	25.3	17.2	13.7	1	1	0	0	1
DR-Retene/C4phe	0.045	0.04	0.04	0.04	0.05	0.04	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.8	1.7	4.2	0.2	1.6	1	1	1	1	1
DR-BaF/4Mpy	0.439	0.45	0.45	0.45	0.45	0.45	0.02	0.02	0.02	0.02	0.02	0.06	0.06	0.06	0.06	0.06	5.2	3.5	3.6	4.0	4.0	1	1	1	1	1
DR-BbcF/4Mpy	0.248	0.26	0.27	0.26	0.27	0.26	0.03	0.03	0.03	0.03	0.03	0.04	0.04	0.04	0.04	0.04	12.5	12.7	11.8	12.9	12.5	1	1	1	1	1
DR-2Mpy/4Mpy	0.957	0.96	0.96	0.96	0.97	0.96	0.00	0.00	0.00	0.02	0.00	0.13	0.13	0.13	0.14	0.13	0.4	0.2	0.3	2.1	0.4	1	1	1	1	1
DR-1Mpy/4Mpy	0.897	0.91	0.91	0.94	0.91	0.92	0.03	0.02	0.08	0.03	0.04	0.13	0.13	0.13	0.13	0.13	3.8	2.6	8.3	3.1	4.5	1	1	1	1	1
DR-SES1/SES2 **m/z123**	1.283	1.45	1.48	1.50	1.50	1.48	0.34	0.39	0.44	0.43	0.40	0.20	0.21	0.21	0.21	0.21	23.2	26.7	29.3	28.9	27.0	0	0	0	0	0
DR-SES3/SES5	0.284	0.37	0.34	0.34	0.35	0.35	0.17	0.11	0.12	0.13	0.13	0.05	0.05	0.05	0.05	0.05	47.0	31.3	34.8	37.6	37.9	0	0	0	0	0
DR-SES4/SES6	0.775	0.91	0.89	0.85	0.87	0.88	0.27	0.22	0.14	0.18	0.21	0.13	0.12	0.12	0.12	0.12	29.9	25.2	16.6	21.3	23.4	0	0	0	0	0
DR-SES5/SES10	0.463	0.68	0.72	0.70	0.70	0.70	0.43	0.52	0.47	0.48	0.47	0.10	0.10	0.10	0.10	0.10	63.7	71.9	67.3	67.9	67.8	0	0	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2007-0017	06-Feb-2007	Emulsion from "TV-bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2. 2007-0023	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 3
3. 2007-0024	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 4
4. 2007-0033	07-Feb-2007	Oil sample collected at KV " Eigun"

Figure E.3: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0068) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007–0017 Test Date: 06–Feb–2007 Description: Emulsion from "TV–bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.

Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR–C28 **m/z191**	0.221	0.22	0.21	0.23	0.23	0.22	0.00	0.01	0.02	0.01	0.00	0.03	0.03	0.03	0.03	0.03	0.0	5.6	8.0	5.9	2.2	1	1	1	1	1
DR–C29	0.164	0.16	0.16	0.17	0.16	0.17	0.00	0.00	0.01	0.00	0.00	0.02	0.02	0.02	0.02	0.02	0.0	0.6	5.9	1.9	0.9	1	1	1	1	1
DR–C28C29	0.385	0.39	0.38	0.40	0.39	0.39	0.00	0.01	0.03	0.01	0.01	0.05	0.05	0.06	0.05	0.05	0.0	3.5	7.1	2.7	1.7	1	1	1	1	1
DR–27Ts	0.515	0.52	0.51	0.53	0.51	0.52	0.00	0.00	0.03	0.01	0.00	0.07	0.07	0.07	0.07	0.07	0.0	0.6	5.2	1.7	0.8	1	1	1	1	1
DR–28ab	0.148	0.15	0.13	0.14	0.14	0.14	0.00	0.03	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.02	0.0	21.4	6.5	7.3	8.5	1	0	1	1	1
DR–25nor30ab	0.068	0.07	0.06	0.06	0.07	0.06	0.00	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.0	20.8	17.1	7.1	10.9	1	0	0	1	1
DR–29Ts	0.164	0.16	0.16	0.16	0.16	0.16	0.00	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.02	0.0	4.2	6.1	4.0	3.5	1	1	1	1	1
DR–30O	0.092	0.09	0.10	0.09	0.09	0.10	0.00	0.02	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.0	22.1	5.4	4.2	5.8	1	0	1	1	1
DR–30G	0.139	0.14	0.13	0.14	0.13	0.13	0.00	0.02	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.02	0.0	16.0	4.3	9.0	7.2	1	0	1	1	1
DR–29ab	0.902	0.90	0.92	0.88	0.91	0.91	0.00	0.04	0.03	0.03	0.01	0.13	0.13	0.12	0.13	0.13	0.0	4.5	3.8	2.8	0.9	1	1	1	1	1
DR–30d	0.054	0.05	0.05	0.05	0.05	0.05	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.0	25.9	23.9	20.8	17.1	1	0	0	0	0
DR–29aaS **m/z217**	0.871	0.87	0.88	0.87	0.89	0.88	0.00	0.02	0.01	0.05	0.01	0.12	0.12	0.12	0.13	0.12	0.0	2.1	0.8	5.1	1.6	1	1	1	1	1
DR–29bb **&218**	0.983	0.98	0.94	0.98	0.95	0.96	0.00	0.09	0.00	0.06	0.04	0.14	0.13	0.14	0.13	0.14	0.0	9.3	0.2	6.5	3.8	1	1	1	1	1
DR–27bbSTER	0.748	0.75	0.74	0.76	0.75	0.75	0.00	0.01	0.02	0.00	0.00	0.10	0.10	0.11	0.10	0.10	0.0	1.0	2.2	0.5	0.2	1	1	1	1	1
DR–28bbSTER	0.307	0.31	0.31	0.31	0.31	0.31	0.00	0.01	0.01	0.00	0.01	0.04	0.04	0.04	0.04	0.04	0.0	2.8	3.3	1.3	1.9	1	1	1	1	1
DR–29bbSTER	0.509	0.51	0.51	0.50	0.51	0.50	0.00	0.01	0.03	0.00	0.01	0.07	0.07	0.07	0.07	0.07	0.0	1.2	5.1	0.4	1.7	1	1	1	1	1
DR–TA21 **m/z231**	4.862	4.86	4.41	4.75	4.73	4.69	0.00	0.90	0.22	0.26	0.35	0.68	0.62	0.67	0.66	0.66	0.0	20.5	4.7	5.6	7.4	1	0	1	1	1
DR–TA26	0.441	0.44	0.46	0.44	0.44	0.44	0.00	0.04	0.00	0.01	0.01	0.06	0.06	0.06	0.06	0.06	0.0	9.0	0.4	2.7	1.6	1	1	1	1	1
DR–TA27	1.031	1.03	1.04	1.02	1.03	1.03	0.00	0.02	0.01	0.01	0.00	0.14	0.15	0.14	0.14	0.14	0.0	1.5	1.2	0.5	0.0	1	1	1	1	1
DR–2MP/1MP **PAH**	2.143	2.14	2.16	2.15	2.15	2.15	0.00	0.03	0.01	0.01	0.01	0.30	0.30	0.30	0.30	0.30	0.0	1.3	0.2	0.5	0.5	1	1	1	1	1
DR–4MD/1MD	2.434	2.43	2.45	2.42	2.44	2.44	0.00	0.03	0.02	0.01	0.00	0.34	0.34	0.34	0.34	0.34	0.0	1.1	0.9	0.4	0.2	1	1	1	1	1
DR–C2dbt/C2phe	0.626	0.63	0.65	0.62	0.63	0.63	0.00	0.04	0.02	0.01	0.01	0.09	0.09	0.09	0.09	0.09	0.0	6.1	2.6	0.8	1.1	1	1	1	1	1
DR–C3dbt/C3phe	0.795	0.80	0.81	0.78	0.79	0.80	0.00	0.04	0.03	0.01	0.00	0.11	0.11	0.11	0.11	0.11	0.0	4.7	3.8	1.3	0.0	1	1	1	1	1
DR–C3dbt/C3chr	2.947	2.95	3.16	2.78	2.89	2.94	0.00	0.42	0.33	0.11	0.01	0.41	0.44	0.39	0.41	0.41	0.0	13.2	11.9	3.7	0.2	1	1	1	1	1
DR–Retene/C4phe	0.045	0.04	0.04	0.04	0.05	0.04	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.0	0.9	3.4	1.0	0.8	1	1	1	1	1
DR–BaF/4Mpy	0.463	0.46	0.46	0.46	0.46	0.46	0.00	0.01	0.01	0.01	0.01	0.06	0.06	0.06	0.06	0.06	0.0	1.8	1.7	1.3	1.2	1	1	1	1	1
DR–BbcF/4Mpy	0.282	0.28	0.28	0.28	0.28	0.28	0.00	0.00	0.00	0.00	0.00	0.04	0.04	0.04	0.04	0.04	0.0	0.2	0.7	0.4	0.0	1	1	1	1	1
DR–2Mpy/4Mpy	0.954	0.95	0.96	0.95	0.97	0.96	0.00	0.01	0.00	0.02	0.01	0.13	0.13	0.13	0.14	0.13	0.0	0.6	0.0	2.4	0.8	1	1	1	1	1
DR–1Mpy/4Mpy	0.932	0.93	0.93	0.95	0.93	0.94	0.00	0.01	0.04	0.01	0.01	0.13	0.13	0.13	0.13	0.13	0.0	1.2	4.5	0.7	0.7	1	1	1	1	1
DR–SES1/SES8 **m/z123**	1.619	1.62	1.65	1.67	1.67	1.65	0.00	0.06	0.10	0.10	0.06	0.23	0.23	0.23	0.23	0.23	0.0	3.5	6.2	5.8	3.9	1	1	1	1	1
DR–SES3/SES5	0.458	0.46	0.42	0.43	0.44	0.44	0.00	0.07	0.05	0.04	0.04	0.06	0.06	0.06	0.06	0.06	0.0	16.3	12.7	9.8	9.5	1	0	1	1	1
DR–SES4/SES6	1.048	1.05	1.02	0.98	1.00	1.01	0.00	0.05	0.13	0.09	0.07	0.15	0.14	0.14	0.14	0.14	0.0	4.8	13.5	8.8	6.7	1	1	1	1	1
DR–SES5/SES10	0.895	0.90	0.94	0.91	0.92	0.92	0.00	0.09	0.04	0.04	0.04	0.13	0.13	0.13	0.13	0.13	0.0	9.3	4.1	4.7	4.6	1	1	1	1	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2007–0017	06–Feb–2007	Emulsion from "TV–bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2. 2007–0023	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 3
3. 2007–0024	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 4
4. 2007–0033	07–Feb–2007	Oil sample collected at KV " Eigun"

Figure E.4: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0017) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007–0025 Test Date: 31–Jan–2007 Description: Oil sample from sandy beach, Selje kommune

Ratio Name		Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
			R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR–C28	**m/z191**	0.165	0.19	0.19	0.20	0.20	0.20	0.06	0.04	0.07	0.07	0.06	0.03	0.03	0.03	0.03	0.03	29.0	23.5	36.8	34.8	31.2	0	0	0	0	0
DR–C29		0.126	0.14	0.14	0.15	0.14	0.15	0.04	0.04	0.05	0.04	0.04	0.02	0.02	0.02	0.02	0.02	26.8	26.2	32.6	25.0	27.7	0	0	0	0	0
DR–C28C29		0.290	0.34	0.33	0.35	0.34	0.34	0.09	0.08	0.12	0.11	0.10	0.05	0.05	0.05	0.05	0.05	28.1	24.7	35.0	30.7	29.7	0	0	0	0	0
DR–27Ts		0.548	0.53	0.53	0.55	0.53	0.53	0.03	0.03	0.00	0.04	0.03	0.07	0.07	0.08	0.07	0.07	6.0	6.6	0.8	7.8	5.3	1	1	1	1	1
DR–28ab		0.096	0.12	0.11	0.12	0.12	0.12	0.05	0.02	0.04	0.04	0.04	0.02	0.02	0.02	0.02	0.02	42.6	21.6	36.3	35.6	34.4	0	0	0	0	0
DR–25nor30ab		0.049	0.06	0.05	0.05	0.06	0.06	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	33.2	12.6	16.3	26.3	22.5	0	1	0	0	0
DR–29Ts		0.163	0.16	0.16	0.16	0.16	0.16	0.00	0.01	0.01	0.01	0.00	0.02	0.02	0.02	0.02	0.02	0.6	3.6	5.5	3.4	3.0	1	1	1	1	1
DR–30O		0.087	0.09	0.10	0.09	0.09	0.09	0.01	0.03	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	6.4	28.4	1.0	10.6	12.2	1	0	1	1	1
DR–30G		0.113	0.13	0.12	0.12	0.12	0.12	0.03	0.01	0.02	0.01	0.02	0.02	0.02	0.02	0.02	0.02	20.8	4.9	16.6	11.9	13.7	0	1	0	1	1
DR–29ab		0.945	0.92	0.94	0.91	0.94	0.93	0.04	0.00	0.08	0.02	0.04	0.13	0.13	0.13	0.13	0.13	4.7	0.2	8.5	1.9	3.8	1	1	1	1	1
DR–30d		0.037	0.05	0.04	0.04	0.04	0.04	0.02	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	37.0	11.5	13.5	16.6	20.3	0	1	1	0	0
DR–29aaS	**m/z217**	0.916	0.89	0.90	0.89	0.92	0.90	0.05	0.03	0.05	0.00	0.03	0.13	0.13	0.12	0.13	0.13	5.1	2.9	5.8	0.0	3.4	1	1	1	1	1
DR–29bb	**&218**	1.013	1.00	0.95	1.00	0.97	0.98	0.03	0.12	0.03	0.09	0.07	0.14	0.13	0.14	0.14	0.14	3.0	12.3	2.8	9.5	6.8	1	1	1	1	1
DR–27bbSTER		0.635	0.69	0.69	0.70	0.69	0.69	0.11	0.11	0.13	0.11	0.11	0.10	0.10	0.10	0.10	0.10	16.4	15.5	18.6	15.9	16.6	0	0	0	0	0
DR–28bbSTER		0.314	0.31	0.31	0.32	0.31	0.31	0.01	0.00	0.00	0.00	0.00	0.04	0.04	0.04	0.04	0.04	2.3	0.4	1.0	1.1	0.5	1	1	1	1	1
DR–29bbSTER		0.594	0.55	0.55	0.54	0.55	0.55	0.09	0.09	0.11	0.09	0.09	0.08	0.08	0.08	0.08	0.08	15.5	16.7	20.5	15.9	17.1	0	0	0	0	0
DR–TA21	**m/z231**	4.020	4.44	3.99	4.33	4.31	4.27	0.84	0.06	0.62	0.58	0.50	0.62	0.56	0.61	0.60	0.60	19.0	1.5	14.3	13.4	11.6	0	1	0	1	1
DR–TA26		0.372	0.41	0.43	0.41	0.40	0.41	0.07	0.11	0.07	0.06	0.08	0.06	0.06	0.06	0.06	0.06	17.0	25.9	16.6	14.3	18.5	0	0	0	0	0
DR–TA27		1.090	1.06	1.07	1.05	1.06	1.06	0.06	0.04	0.07	0.06	0.06	0.15	0.15	0.15	0.15	0.15	5.6	4.1	6.8	6.1	5.6	1	1	1	1	1
DR–2MP/1MP	**PAH**	2.094	2.12	2.13	2.12	2.12	2.12	0.05	0.08	0.05	0.06	0.06	0.30	0.30	0.30	0.30	0.30	2.3	3.7	2.6	2.8	2.9	1	1	1	1	1
DR–4MD/1MD		2.510	2.47	2.49	2.46	2.48	2.47	0.08	0.05	0.10	0.07	0.07	0.35	0.35	0.34	0.35	0.35	3.1	2.0	3.9	2.6	2.9	1	1	1	1	1
DR–C2dbt/C2phe		0.648	0.64	0.66	0.63	0.64	0.64	0.02	0.02	0.04	0.02	0.02	0.09	0.09	0.09	0.09	0.09	3.5	2.6	6.2	2.7	2.4	1	1	1	1	1
DR–C3dbt/C3phe		0.811	0.80	0.82	0.79	0.80	0.80	0.02	0.02	0.05	0.03	0.02	0.11	0.12	0.11	0.11	0.11	1.9	2.8	5.7	3.3	2.0	1	1	1	1	1
DR–C3dbt/C3chr		2.924	2.94	3.14	2.77	2.88	2.93	0.02	0.44	0.31	0.08	0.02	0.41	0.44	0.39	0.40	0.41	0.8	14.0	11.1	2.9	0.6	1	0	1	1	1
DR–Retene/C4phe		0.052	0.05	0.05	0.05	0.05	0.05	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	15.4	16.3	18.8	14.4	16.2	0	0	0	0	0
DR–BaF/4Mpy		0.434	0.45	0.44	0.44	0.45	0.45	0.03	0.02	0.02	0.02	0.02	0.06	0.06	0.06	0.06	0.06	6.3	4.5	4.6	5.1	5.1	1	1	1	1	1
DR–BbcF/4Mpy		0.234	0.26	0.26	0.26	0.26	0.26	0.05	0.05	0.05	0.05	0.05	0.04	0.04	0.04	0.04	0.04	18.5	18.7	17.8	18.9	18.5	0	0	0	0	0
DR–2Mpy/4Mpy		0.940	0.95	0.95	0.95	0.96	0.95	0.01	0.02	0.01	0.04	0.02	0.13	0.13	0.13	0.13	0.13	1.5	2.0	1.5	3.9	2.2	1	1	1	1	1
DR–1Mpy/4Mpy		0.950	0.94	0.94	0.96	0.94	0.94	0.02	0.03	0.03	0.02	0.01	0.13	0.13	0.13	0.13	0.13	1.9	3.1	2.6	2.5	1.2	1	1	1	1	1
DR–SES1/SES8	**m/z123**	1.470	1.54	1.57	1.60	1.59	1.58	0.15	0.21	0.25	0.25	0.21	0.22	0.22	0.22	0.22	0.22	9.6	13.2	15.8	15.4	13.5	1	1	0	0	1
DR–SES3/SES5		0.364	0.41	0.38	0.38	0.39	0.39	0.09	0.02	0.04	0.05	0.05	0.06	0.05	0.05	0.05	0.05	22.9	6.6	10.3	13.2	13.4	0	1	1	1	1
DR–SES4/SES6		0.810	0.93	0.90	0.86	0.89	0.90	0.24	0.19	0.11	0.15	0.17	0.13	0.13	0.12	0.12	0.13	25.6	20.9	12.2	16.9	19.0	0	0	1	0	0
DR–SES5/SES10		0.559	0.73	0.77	0.75	0.75	0.75	0.34	0.42	0.37	0.38	0.38	0.10	0.11	0.10	0.10	0.10	46.3	55.0	50.1	50.7	50.6	0	0	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2007–0017	06–Feb–2007	Emulsion from "TV–bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2. 2007–0023	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 3
3. 2007–0024	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 4
4. 2007–0033	07–Feb–2007	Oil sample collected at KV " Eigun"

Figure E.5: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0025) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007–0070 Test Date: 09–Aug–2007 Description: Bird feathers from wounded seagull (skårunge), Træna

Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR–C28 **m/z191**	0.102	0.16	0.16	0.17	0.17	0.16	0.12	0.11	0.14	0.13	0.12	0.02	0.02	0.02	0.02	0.02	73.3	68.3	80.1	78.3	75.2	0	0	0	0	0
DR–C29	0.109	0.14	0.14	0.14	0.14	0.14	0.05	0.05	0.06	0.05	0.06	0.02	0.02	0.02	0.02	0.02	40.1	39.5	45.7	38.4	41.0	0	0	0	0	0
DR–C28C29	0.212	0.30	0.29	0.31	0.30	0.30	0.17	0.16	0.20	0.18	0.18	0.04	0.04	0.04	0.04	0.04	58.1	54.9	64.5	60.5	59.6	0	0	0	0	0
DR–27Ts	0.672	0.59	0.59	0.61	0.59	0.60	0.16	0.16	0.13	0.17	0.15	0.08	0.08	0.09	0.08	0.08	26.3	26.9	21.2	28.0	25.6	0	0	0	0	0
DR–28ab	0.000	0.07	0.06	0.07	0.07	0.07	0.15	0.12	0.14	0.14	0.14	0.01	0.01	0.01	0.01	0.01	200.0	200.0	200.0	200.0	200.0	0	0	0	0	0
DR–25nor30ab	0.040	0.05	0.05	0.05	0.05	0.05	0.03	0.02	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.01	51.3	31.3	35.0	44.6	40.9	0	0	0	0	0
DR–29Ts	0.170	0.17	0.16	0.16	0.16	0.16	0.01	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.02	3.2	7.4	9.2	7.1	6.7	1	1	1	1	1
DR–30O	0.018	0.05	0.07	0.05	0.06	0.06	0.07	0.10	0.07	0.08	0.08	0.01	0.01	0.01	0.01	0.01	136.2	147.2	133.2	138.4	139.2	0	0	0	0	0
DR–30G	0.088	0.11	0.10	0.11	0.11	0.11	0.05	0.03	0.05	0.04	0.04	0.02	0.01	0.02	0.02	0.02	45.0	29.5	40.9	36.4	38.2	0	0	0	0	0
DR–29ab	0.818	0.86	0.88	0.84	0.87	0.86	0.08	0.12	0.05	0.11	0.09	0.12	0.12	0.12	0.12	0.12	9.7	14.2	5.9	12.5	10.6	1	0	1	1	1
DR–30d	0.049	0.05	0.05	0.05	0.05	0.05	0.01	0.01	0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.01	10.9	15.0	13.0	9.9	6.2	1	0	1	1	1
DR–29aaS **m/z217**	0.914	0.89	0.90	0.89	0.91	0.90	0.04	0.02	0.05	0.00	0.03	0.12	0.13	0.12	0.13	0.13	4.8	2.7	5.6	0.2	3.2	1	1	1	1	1
DR–29bb **&218**	1.073	1.03	0.98	1.03	1.00	1.01	0.09	0.18	0.09	0.15	0.13	0.14	0.14	0.14	0.14	0.14	8.7	18.0	8.5	15.2	12.5	1	0	1	0	1
DR–27bbSTER	0.532	0.64	0.64	0.65	0.64	0.64	0.22	0.21	0.23	0.21	0.22	0.09	0.09	0.09	0.09	0.09	33.7	32.7	35.8	33.1	33.8	0	0	0	0	0
DR–28bbSTER	0.340	0.32	0.33	0.33	0.33	0.33	0.03	0.02	0.02	0.03	0.03	0.05	0.05	0.05	0.05	0.05	10.3	7.5	7.0	9.0	8.5	1	1	1	1	1
DR–29bbSTER	0.663	0.59	0.58	0.57	0.58	0.58	0.15	0.16	0.18	0.16	0.16	0.08	0.08	0.08	0.08	0.08	26.3	27.5	31.3	26.7	28.0	0	0	0	0	0
DR–TA21 **m/z231**	0.468	2.67	2.21	2.55	2.53	2.49	4.39	3.49	4.17	4.13	4.05	0.37	0.31	0.36	0.35	0.35	164.9	157.7	163.4	163.1	162.4	0	0	0	0	0
DR–TA26	0.413	0.43	0.45	0.43	0.42	0.43	0.03	0.07	0.03	0.02	0.04	0.06	0.06	0.06	0.06	0.06	6.6	15.5	6.2	3.8	8.1	1	0	1	1	1
DR–TA27	0.732	0.88	0.89	0.88	0.88	0.88	0.30	0.31	0.29	0.29	0.30	0.12	0.12	0.12	0.12	0.12	33.9	35.4	32.8	33.4	33.9	0	0	0	0	0
DR–2MP/1MP **PAH**	2.248	2.20	2.21	2.20	2.20	2.20	0.10	0.08	0.10	0.09	0.09	0.31	0.31	0.31	0.31	0.31	4.8	3.4	4.5	4.3	4.3	1	1	1	1	1
DR–4MD/1MD	2.929	2.68	2.70	2.67	2.69	2.68	0.49	0.47	0.52	0.48	0.49	0.38	0.38	0.37	0.38	0.38	18.5	17.4	19.3	18.0	18.3	0	0	0	0	0
DR–C2dbt/C2phe	0.307	0.47	0.49	0.46	0.47	0.47	0.32	0.36	0.30	0.32	0.33	0.07	0.07	0.06	0.07	0.07	68.5	73.8	66.2	69.2	69.5	0	0	0	0	0
DR–C3dbt/C3phe	0.400	0.60	0.62	0.58	0.59	0.60	0.40	0.43	0.37	0.38	0.39	0.08	0.09	0.08	0.08	0.08	66.1	70.3	62.7	64.9	66.0	0	0	0	0	0
DR–C3dbt/C3chr	1.415	2.18	2.39	2.02	2.13	2.18	1.53	1.95	1.20	1.43	1.53	0.31	0.33	0.28	0.30	0.30	70.3	81.6	59.6	67.0	70.1	0	0	0	0	0
DR–Retene/C4phe	0.056	0.05	0.05	0.05	0.05	0.05	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	22.6	23.5	26.0	21.6	23.4	0	0	0	0	0
DR–BaF/4Mpy	0.560	0.51	0.51	0.51	0.51	0.51	0.10	0.11	0.10	0.10	0.10	0.07	0.07	0.07	0.07	0.07	19.0	20.7	20.6	20.2	20.1	0	0	0	0	0
DR–BbcF/4Mpy	0.284	0.28	0.28	0.28	0.28	0.28	0.00	0.00	0.00	0.00	0.00	0.04	0.04	0.04	0.04	0.04	0.9	0.7	1.6	0.5	0.9	1	1	1	1	1
DR–2Mpy/4Mpy	0.947	0.95	0.95	0.95	0.96	0.95	0.01	0.01	0.01	0.03	0.01	0.13	0.13	0.13	0.13	0.13	0.7	1.3	0.8	3.2	1.5	1	1	1	1	1
DR–1Mpy/4Mpy	0.913	0.92	0.92	0.94	0.92	0.93	0.02	0.01	0.06	0.01	0.03	0.13	0.13	0.13	0.13	0.13	2.1	0.9	6.6	1.4	2.8	1	1	1	1	1
DR–SES1/SES2 **m/z123**	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0	0	0
DR–SES3/SES5	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0	0	0
DR–SES4/SES6	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0	0	0
DR–SES5/SES10	0.000	0.45	0.49	0.47	0.47	0.47	0.90	0.98	0.93	0.94	0.94	0.06	0.07	0.07	0.07	0.07	200.0	200.0	200.0	200.0	200.0	0	0	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2007–0017	06–Feb–2007	Emulsion from "TV–bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2. 2007–0023	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 3
3. 2007–0024	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 4
4. 2007–0033	07–Feb–2007	Oil sample collected at KV " Eigun"

Figure E.6: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0070) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007-0033 Test Date: 07-Feb-2007 Description: Oil sample collected at KV " Eigun"

Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR-C28 **m/z191**	0.234	0.23	0.22	0.24	0.23	0.23	0.01	0.03	0.01	0.00	0.01	0.03	0.03	0.03	0.03	0.03	5.9	11.5	2.1	0.0	3.7	1	1	1	1	1
DR-C29	0.161	0.16	0.16	0.17	0.16	0.16	0.00	0.00	0.01	0.00	0.00	0.02	0.02	0.02	0.02	0.02	1.9	1.2	7.7	0.0	2.7	1	1	1	1	1
DR-C28C29	0.396	0.39	0.38	0.40	0.40	0.39	0.01	0.02	0.02	0.00	0.00	0.05	0.05	0.06	0.06	0.06	2.7	6.1	4.4	0.0	1.0	1	1	1	1	1
DR-27Ts	0.507	0.51	0.51	0.52	0.51	0.51	0.01	0.01	0.04	0.00	0.01	0.07	0.07	0.07	0.07	0.07	1.7	1.2	6.9	0.0	2.5	1	1	1	1	1
DR-28ab	0.137	0.14	0.13	0.14	0.14	0.14	0.01	0.02	0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.02	7.3	14.2	0.8	0.0	1.2	1	0	1	1	1
DR-25nor30ab	0.064	0.07	0.06	0.06	0.06	0.06	0.00	0.01	0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.01	7.1	13.8	10.0	0.0	3.8	1	1	1	1	1
DR-29Ts	0.158	0.16	0.16	0.16	0.16	0.16	0.01	0.00	0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.02	4.0	0.2	2.1	0.0	0.5	1	1	1	1	1
DR-30O	0.096	0.09	0.11	0.09	0.10	0.10	0.00	0.02	0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.01	4.2	17.9	9.6	0.0	1.6	1	0	1	1	1
DR-30G	0.127	0.13	0.12	0.13	0.13	0.13	0.01	0.01	0.01	0.00	0.00	0.02	0.02	0.02	0.02	0.02	9.0	7.0	4.7	0.0	1.8	1	1	1	1	1
DR-29ab	0.927	0.91	0.94	0.90	0.93	0.92	0.03	0.02	0.06	0.00	0.02	0.13	0.13	0.13	0.13	0.13	2.8	1.7	6.6	0.0	1.9	1	1	1	1	1
DR-30d	0.044	0.05	0.04	0.04	0.04	0.04	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	20.8	5.1	3.1	0.0	3.7	0	1	1	1	1
DR-29aaS **m/z217**	0.916	0.89	0.90	0.89	0.92	0.90	0.05	0.03	0.05	0.00	0.03	0.13	0.13	0.12	0.13	0.13	5.1	2.9	5.8	0.0	3.4	1	1	1	1	1
DR-29bb **&218**	0.921	0.95	0.91	0.95	0.92	0.93	0.06	0.02	0.06	0.00	0.03	0.13	0.13	0.13	0.13	0.13	6.5	2.8	6.7	0.0	2.7	1	1	1	1	1
DR-27bbSTER	0.744	0.75	0.74	0.75	0.74	0.75	0.00	0.00	0.02	0.00	0.01	0.10	0.10	0.11	0.10	0.10	0.5	0.4	2.7	0.0	0.7	1	1	1	1	1
DR-28bbSTER	0.311	0.31	0.31	0.31	0.31	0.31	0.00	0.00	0.01	0.00	0.00	0.04	0.04	0.04	0.04	0.04	1.3	1.5	2.0	0.0	0.6	1	1	1	1	1
DR-29bbSTER	0.507	0.51	0.50	0.50	0.51	0.50	0.00	0.00	0.02	0.00	0.01	0.07	0.07	0.07	0.07	0.07	0.4	0.8	4.7	0.0	1.2	1	1	1	1	1
DR-TA21 **m/z231**	4.600	4.73	4.28	4.62	4.60	4.56	0.26	0.64	0.04	0.00	0.08	0.66	0.60	0.65	0.64	0.64	5.6	15.0	0.9	0.0	1.8	1	0	1	1	1
DR-TA26	0.430	0.44	0.46	0.43	0.43	0.44	0.01	0.05	0.01	0.00	0.02	0.06	0.06	0.06	0.06	0.06	2.7	11.7	2.4	0.0	4.3	1	1	1	1	1
DR-TA27	1.025	1.03	1.04	1.02	1.03	1.03	0.01	0.02	0.01	0.00	0.00	0.14	0.15	0.14	0.14	0.14	0.5	2.0	0.7	0.0	0.5	1	1	1	1	1
DR-2MP/1MP **PAH**	2.153	2.15	2.16	2.15	2.15	2.15	0.01	0.02	0.00	0.00	0.00	0.30	0.30	0.30	0.30	0.30	0.5	0.9	0.2	0.0	0.1	1	1	1	1	1
DR-4MD/1MD	2.444	2.44	2.45	2.43	2.44	2.44	0.01	0.02	0.03	0.00	0.01	0.34	0.34	0.34	0.34	0.34	0.4	0.7	1.3	0.0	0.3	1	1	1	1	1
DR-C2dbt/C2phe	0.631	0.63	0.65	0.62	0.63	0.63	0.01	0.03	0.02	0.00	0.00	0.09	0.09	0.09	0.09	0.09	0.8	5.3	3.5	0.0	0.3	1	1	1	1	1
DR-C3dbt/C3phe	0.785	0.79	0.81	0.78	0.78	0.79	0.01	0.05	0.02	0.00	0.01	0.11	0.11	0.11	0.11	0.11	1.3	6.1	2.5	0.0	1.3	1	1	1	1	1
DR-C3dbt/C3chr	2.840	2.89	3.10	2.73	2.84	2.89	0.11	0.52	0.22	0.00	0.10	0.41	0.43	0.38	0.40	0.40	3.7	16.9	8.2	0.0	3.5	1	0	1	1	1
DR-Retene/C4phe	0.045	0.05	0.04	0.04	0.05	0.04	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	1.0	1.9	4.4	0.0	1.8	1	1	1	1	1
DR-BaF/4Mpy	0.457	0.46	0.46	0.46	0.46	0.46	0.01	0.00	0.00	0.00	0.00	0.06	0.06	0.06	0.06	0.06	1.3	0.5	0.4	0.0	0.1	1	1	1	1	1
DR-BbcF/4Mpy	0.283	0.28	0.28	0.28	0.28	0.28	0.00	0.00	0.00	0.00	0.00	0.04	0.04	0.04	0.04	0.04	0.4	0.2	1.1	0.0	0.4	1	1	1	1	1
DR-2Mpy/4Mpy	0.977	0.97	0.97	0.97	0.98	0.97	0.02	0.02	0.02	0.00	0.02	0.14	0.14	0.14	0.14	0.14	2.4	1.8	2.4	0.0	1.7	1	1	1	1	1
DR-1Mpy/4Mpy	0.926	0.93	0.92	0.95	0.93	0.93	0.01	0.00	0.05	0.00	0.01	0.13	0.13	0.13	0.13	0.13	0.7	0.5	5.2	0.0	1.4	1	1	1	1	1
DR-SES1/SES2 **m/z123**	1.716	1.67	1.70	1.72	1.72	1.70	0.10	0.04	0.01	0.00	0.03	0.23	0.24	0.24	0.24	0.24	5.8	2.2	0.4	0.0	1.9	1	1	1	1	1
DR-SES3/SES5	0.415	0.44	0.40	0.41	0.41	0.42	0.04	0.03	0.01	0.00	0.00	0.06	0.06	0.06	0.06	0.06	9.8	6.5	2.9	0.0	0.3	1	1	1	1	1
DR-SES4/SES6	0.960	1.00	0.98	0.94	0.96	0.97	0.09	0.04	0.04	0.00	0.02	0.14	0.14	0.13	0.13	0.14	8.8	4.0	4.8	0.0	2.1	1	1	1	1	1
DR-SES5/SES10	0.939	0.92	0.96	0.94	0.94	0.94	0.04	0.04	0.01	0.00	0.00	0.13	0.13	0.13	0.13	0.13	4.7	4.6	0.6	0.0	0.1	1	1	1	1	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2007-0017	06-Feb-2007	Emulsion from "TV-bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2. 2007-0023	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 3
3. 2007-0024	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 4
4. 2007-0033	07-Feb-2007	Oil sample collected at KV " Eigun"

Figure E.7: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0033) and the reference samples.

Evaluation of The Diagnostic Ratio - MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007-0062 Test Date: 06-Feb-2007 Description: Oil on birds (gulls)Onøy, Lurøy

Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR-C28 **m/z191**	0.092	0.16	0.15	0.17	0.16	0.16	0.13	0.12	0.15	0.14	0.13	0.02	0.02	0.02	0.02	0.02	82.6	77.9	89.2	87.5	84.4	0	0	0	0	0
DR-C29	0.108	0.14	0.14	0.14	0.13	0.14	0.06	0.06	0.07	0.05	0.06	0.02	0.02	0.02	0.02	0.02	41.8	41.2	47.4	40.0	42.7	0	0	0	0	0
DR-C28C29	0.199	0.29	0.29	0.31	0.30	0.30	0.19	0.17	0.21	0.20	0.19	0.04	0.04	0.04	0.04	0.04	63.6	60.5	70.0	66.0	65.1	0	0	0	0	0
DR-27Ts	0.606	0.56	0.56	0.57	0.56	0.56	0.09	0.09	0.06	0.10	0.09	0.08	0.08	0.08	0.08	0.08	16.1	16.6	10.9	17.8	15.3	0	0	1	0	0
DR-28ab	0.042	0.09	0.08	0.09	0.09	0.09	0.11	0.08	0.10	0.10	0.09	0.01	0.01	0.01	0.01	0.01	111.3	95.6	106.8	106.2	105.3	0	0	0	0	0
DR-25nor30ab	0.037	0.05	0.05	0.05	0.05	0.05	0.03	0.02	0.02	0.03	0.02	0.01	0.01	0.01	0.01	0.01	58.4	38.7	42.3	51.8	48.2	0	0	0	0	0
DR-29Ts	0.159	0.16	0.16	0.16	0.16	0.16	0.01	0.00	0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.02	3.2	1.0	2.8	0.8	0.3	1	1	1	1	1
DR-30O	0.018	0.06	0.07	0.05	0.06	0.06	0.07	0.10	0.07	0.08	0.08	0.01	0.01	0.01	0.01	0.01	134.5	145.8	131.5	136.8	137.6	0	0	0	0	0
DR-30G	0.079	0.11	0.10	0.11	0.10	0.10	0.06	0.04	0.05	0.05	0.05	0.02	0.01	0.01	0.01	0.01	54.9	39.7	50.9	46.4	48.2	0	0	0	0	0
DR-29ab	0.753	0.83	0.85	0.81	0.84	0.83	0.15	0.19	0.12	0.17	0.16	0.12	0.12	0.11	0.12	0.12	18.0	22.5	14.3	20.8	18.9	0	0	0	0	0
DR-30d	0.043	0.05	0.04	0.04	0.04	0.04	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	22.2	3.7	1.7	1.4	5.2	0	1	1	1	1
DR-29aaS **m/z217**	0.969	0.92	0.93	0.92	0.94	0.93	0.10	0.08	0.10	0.05	0.08	0.13	0.13	0.13	0.13	0.13	10.7	8.5	11.4	5.6	9.0	1	1	1	1	1
DR-29bb **&218**	1.064	1.02	0.98	1.02	0.99	1.00	0.08	0.17	0.08	0.14	0.12	0.14	0.14	0.14	0.14	0.14	7.9	17.1	7.7	14.4	11.7	1	0	1	0	1
DR-27bbSTER	0.514	0.63	0.63	0.64	0.63	0.63	0.23	0.23	0.25	0.23	0.24	0.09	0.09	0.09	0.09	0.09	37.1	36.1	39.1	36.5	37.2	0	0	0	0	0
DR-28bbSTER	0.334	0.32	0.32	0.33	0.32	0.32	0.03	0.02	0.02	0.02	0.02	0.04	0.05	0.05	0.05	0.05	8.4	5.6	5.1	7.1	6.6	1	1	1	1	1
DR-29bbSTER	0.695	0.60	0.60	0.59	0.60	0.60	0.19	0.19	0.21	0.19	0.19	0.08	0.08	0.08	0.08	0.08	30.9	32.1	35.9	31.4	32.6	0	0	0	0	0
DR-TA21 **m/z231**	0.987	2.92	2.47	2.81	2.79	2.75	3.88	2.97	3.65	3.61	3.53	0.41	0.35	0.39	0.39	0.39	132.5	120.2	129.9	129.3	128.3	0	0	0	0	0
DR-TA26	0.400	0.42	0.44	0.42	0.41	0.42	0.04	0.08	0.04	0.03	0.05	0.06	0.06	0.06	0.06	0.06	9.8	18.8	9.5	7.1	11.4	1	0	1	1	1
DR-TA27	0.788	0.91	0.92	0.90	0.91	0.91	0.24	0.26	0.23	0.24	0.24	0.13	0.13	0.13	0.13	0.13	26.8	28.2	25.6	26.2	26.7	0	0	0	0	0
DR-2MP/1MP **PAH**	2.197	2.17	2.18	2.17	2.17	2.18	0.05	0.02	0.05	0.04	0.04	0.30	0.31	0.30	0.30	0.30	2.5	1.1	2.2	2.0	1.9	1	1	1	1	1
DR-4MD/1MD	2.941	2.69	2.70	2.68	2.69	2.69	0.51	0.48	0.53	0.50	0.50	0.38	0.38	0.37	0.38	0.38	18.9	17.8	19.7	18.4	18.7	0	0	0	0	0
DR-C2dbt/C2phe	0.293	0.46	0.48	0.45	0.46	0.46	0.33	0.37	0.32	0.34	0.34	0.06	0.07	0.06	0.06	0.06	72.5	77.7	70.2	73.2	73.4	0	0	0	0	0
DR-C3dbt/C3phe	0.374	0.58	0.60	0.57	0.58	0.58	0.42	0.46	0.39	0.41	0.42	0.08	0.08	0.08	0.08	0.08	72.0	76.1	68.7	70.8	72.0	0	0	0	0	0
DR-C3dbt/C3chr	1.868	2.41	2.62	2.24	2.35	2.40	1.08	1.50	0.75	0.97	1.07	0.34	0.37	0.31	0.33	0.34	44.8	57.2	33.4	41.3	44.7	0	0	0	0	0
DR-Retene/C4phe	0.048	0.05	0.05	0.05	0.05	0.05	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	6.2	7.1	9.6	5.2	7.0	1	1	1	1	1
DR-BaF/4Mpy	0.592	0.53	0.52	0.52	0.52	0.52	0.13	0.14	0.14	0.13	0.13	0.07	0.07	0.07	0.07	0.07	24.4	26.2	26.1	25.7	25.6	0	0	0	0	0
DR-BbcF/4Mpy	0.308	0.29	0.30	0.29	0.30	0.29	0.03	0.03	0.03	0.03	0.03	0.04	0.04	0.04	0.04	0.04	9.0	8.8	9.7	8.6	9.0	1	1	1	1	1
DR-2Mpy/4Mpy	0.973	0.96	0.97	0.96	0.98	0.97	0.02	0.01	0.02	0.00	0.01	0.13	0.14	0.13	0.14	0.14	2.0	1.4	2.0	0.4	1.2	1	1	1	1	1
DR-1Mpy/4Mpy	0.879	0.91	0.90	0.93	0.90	0.91	0.05	0.04	0.10	0.05	0.06	0.13	0.13	0.13	0.13	0.13	5.9	4.7	10.4	5.2	6.6	1	1	1	1	1
DR-SES1/SES8 **m/z123**	1.795	1.71	1.74	1.76	1.76	1.74	0.18	0.12	0.07	0.08	0.11	0.24	0.24	0.25	0.25	0.24	10.3	6.8	4.1	4.5	6.4	1	1	1	1	1
DR-SES3/SES5	0.184	0.32	0.29	0.29	0.30	0.30	0.27	0.20	0.22	0.23	0.23	0.04	0.04	0.04	0.04	0.04	85.4	71.6	74.7	77.2	77.4	0	0	0	0	0
DR-SES4/SES6	0.664	0.86	0.83	0.79	0.81	0.82	0.38	0.34	0.25	0.30	0.32	0.12	0.12	0.11	0.11	0.12	45.0	40.4	31.9	36.5	38.6	0	0	0	0	0
DR-SES5/SES10	0.543	0.72	0.76	0.74	0.74	0.74	0.35	0.44	0.39	0.40	0.39	0.10	0.11	0.10	0.10	0.10	48.9	57.6	52.8	53.3	53.2	0	0	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2007-0017	06-Feb-2007	Emulsion from "TV-bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2. 2007-0023	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 3
3. 2007-0024	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 4
4. 2007-0033	07-Feb-2007	Oil sample collected at KV " Eigun"

Figure E.8: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0062) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007-0105 Test Date: 09-Aug-2007 Description: Oil sample from Eide, 9380 Gryllefjord

Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR-C28 **m/z191**	0.151	0.19	0.18	0.19	0.19	0.19	0.07	0.06	0.09	0.08	0.07	0.03	0.03	0.03	0.03	0.03	37.6	32.2	45.3	43.3	39.8	0	0	0	0	0
DR-C29	0.150	0.16	0.16	0.16	0.16	0.16	0.01	0.01	0.02	0.01	0.02	0.02	0.02	0.02	0.02	0.02	9.4	8.7	15.2	7.5	10.3	1	1	0	1	1
DR-C28C29	0.300	0.34	0.34	0.36	0.35	0.35	0.08	0.07	0.11	0.10	0.09	0.05	0.05	0.05	0.05	0.05	24.7	21.3	31.7	27.3	26.3	0	0	0	0	0
DR-27Ts	0.297	0.41	0.40	0.42	0.40	0.41	0.22	0.22	0.25	0.21	0.22	0.06	0.06	0.06	0.06	0.06	53.9	53.4	58.7	52.3	54.6	0	0	0	0	0
DR-28ab	0.000	0.07	0.06	0.07	0.07	0.07	0.15	0.12	0.14	0.14	0.14	0.01	0.01	0.01	0.01	0.01	200.0	200.0	200.0	200.0	200.0	0	0	0	0	0
DR-25nor30ab	0.077	0.07	0.07	0.07	0.07	0.07	0.01	0.02	0.02	0.01	0.02	0.01	0.01	0.01	0.01	0.01	11.3	31.9	28.3	18.4	22.2	1	0	0	0	0
DR-29Ts	0.117	0.14	0.14	0.14	0.14	0.14	0.05	0.04	0.04	0.04	0.04	0.02	0.02	0.02	0.02	0.02	33.4	29.3	27.5	29.5	29.9	0	0	0	0	0
DR-30O	0.030	0.06	0.07	0.06	0.06	0.06	0.06	0.08	0.06	0.07	0.07	0.01	0.01	0.01	0.01	0.01	101.1	116.7	97.0	104.2	105.4	0	0	0	0	0
DR-30G	0.080	0.11	0.10	0.11	0.10	0.10	0.06	0.04	0.05	0.05	0.05	0.02	0.01	0.01	0.01	0.01	54.5	39.4	50.5	46.1	47.8	0	0	0	0	0
DR-29ab	0.821	0.86	0.88	0.84	0.87	0.87	0.08	0.12	0.05	0.11	0.09	0.12	0.12	0.12	0.12	0.12	9.4	13.9	5.6	12.2	10.3	1	1	1	1	1
DR-30d	0.053	0.05	0.05	0.05	0.05	0.05	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	3.3	22.6	20.6	17.6	13.9	1	0	0	0	1
DR-29aaS **m/z217**	1.004	0.94	0.95	0.93	0.96	0.94	0.13	0.11	0.14	0.09	0.12	0.13	0.13	0.13	0.13	0.13	14.2	12.1	15.0	9.2	12.6	0	1	0	1	1
DR-29bb **&218**	0.903	0.94	0.90	0.94	0.91	0.92	0.08	0.01	0.08	0.02	0.04	0.13	0.13	0.13	0.13	0.13	8.5	0.8	8.7	2.0	4.7	1	1	1	1	1
DR-27bbSTER	0.634	0.69	0.69	0.70	0.69	0.69	0.11	0.11	0.13	0.11	0.12	0.10	0.10	0.10	0.10	0.10	16.5	15.6	18.7	16.0	16.7	0	0	0	0	0
DR-28bbSTER	0.388	0.35	0.35	0.35	0.35	0.35	0.08	0.07	0.07	0.08	0.08	0.05	0.05	0.05	0.05	0.05	23.4	20.6	20.1	22.1	21.6	0	0	0	0	0
DR-29bbSTER	0.498	0.50	0.50	0.49	0.50	0.50	0.01	0.00	0.01	0.01	0.00	0.07	0.07	0.07	0.07	0.07	2.2	1.0	2.9	1.7	0.5	1	1	1	1	1
DR-TA21 **m/z231**	1.660	3.26	2.81	3.15	3.13	3.09	3.20	2.30	2.98	2.94	2.86	0.46	0.39	0.44	0.44	0.43	98.2	81.8	94.6	93.9	92.5	0	0	0	0	0
DR-TA26	0.960	0.70	0.72	0.70	0.69	0.70	0.52	0.48	0.52	0.53	0.51	0.10	0.10	0.10	0.10	0.10	74.0	66.1	74.3	76.3	72.6	0	0	0	0	0
DR-TA27	1.182	1.11	1.11	1.10	1.10	1.11	0.15	0.14	0.16	0.16	0.15	0.15	0.16	0.15	0.15	0.15	13.7	12.2	14.9	14.2	13.7	1	1	0	0	1
DR-2MP/1MP **PAH**	2.276	2.21	2.22	2.21	2.21	2.22	0.13	0.10	0.13	0.12	0.12	0.31	0.31	0.31	0.31	0.31	6.0	4.7	5.7	5.5	5.5	1	1	1	1	1
DR-4MD/1MD	2.671	2.55	2.57	2.54	2.56	2.55	0.24	0.21	0.26	0.23	0.23	0.36	0.36	0.36	0.36	0.36	9.3	8.2	10.1	8.8	9.1	1	1	1	1	1
DR-C2dbt/C2phe	0.221	0.42	0.44	0.42	0.43	0.43	0.40	0.44	0.39	0.41	0.41	0.06	0.06	0.06	0.06	0.06	95.6	100.2	93.5	96.2	96.4	0	0	0	0	0
DR-C3dbt/C3phe	0.306	0.55	0.57	0.54	0.55	0.55	0.49	0.53	0.46	0.48	0.49	0.08	0.08	0.08	0.08	0.08	88.9	92.7	85.9	87.8	88.9	0	0	0	0	0
DR-C3dbt/C3chr	1.931	2.44	2.65	2.27	2.39	2.44	1.02	1.43	0.68	0.91	1.01	0.34	0.37	0.32	0.33	0.34	41.6	54.1	30.1	38.1	41.5	0	0	0	0	0
DR-Retene/C4phe	0.045	0.04	0.04	0.04	0.05	0.04	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.2	1.1	3.6	0.8	1.0	1	1	1	1	1
DR-BaF/4Mpy	0.415	0.44	0.43	0.44	0.44	0.44	0.05	0.04	0.04	0.04	0.04	0.06	0.06	0.06	0.06	0.06	10.9	9.1	9.2	9.6	9.7	1	1	1	1	1
DR-BbcF/4Mpy	0.239	0.26	0.26	0.26	0.26	0.26	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	16.4	16.6	15.7	16.8	16.4	0	0	0	0	0
DR-2Mpy/4Mpy	0.972	0.96	0.97	0.96	0.97	0.97	0.02	0.01	0.02	0.01	0.01	0.13	0.14	0.13	0.14	0.14	1.8	1.3	1.8	0.6	1.1	1	1	1	1	1
DR-1Mpy/4Mpy	0.880	0.91	0.90	0.93	0.90	0.91	0.05	0.04	0.09	0.05	0.06	0.13	0.13	0.13	0.13	0.13	5.7	4.5	10.2	5.0	6.4	1	1	1	1	1
DR-SES1/SES2 **m/z123**	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0	0	0
DR-SES3/SES5	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0	0	0
DR-SES4/SES6	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	Inf	NaN	NaN	NaN	NaN	NaN	0	0	0	0	0
DR-SES5/SES10	0.000	0.45	0.49	0.47	0.47	0.47	0.90	0.98	0.93	0.94	0.94	0.06	0.07	0.07	0.07	0.07	200.0	200.0	200.0	200.0	200.0	0	0	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2007-0017	06-Feb-2007	Emulsion from "TV-bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2. 2007-0023	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 3
3. 2007-0024	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 4
4. 2007-0033	07-Feb-2007	Oil sample collected at KV " Eigun"

Figure E.9: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0105) and the reference samples.

Evaluation of The Diagnostic Ratio − MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007−0018 Test Date: 15−Jan−2007 Description: Sample included Teflon pad, Herdla Vest

Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR−C28 **m/z191**	0.259	0.24	0.23	0.25	0.25	0.24	0.04	0.05	0.02	0.02	0.03	0.03	0.03	0.03	0.03	0.03	16.0	21.6	8.0	10.1	13.8	0	0	1	1	1
DR−C29	0.192	0.18	0.18	0.18	0.18	0.18	0.03	0.03	0.02	0.03	0.03	0.02	0.02	0.03	0.02	0.03	15.4	16.0	9.5	17.2	14.5	0	0	1	0	0
DR−C28C29	0.451	0.42	0.41	0.43	0.42	0.42	0.07	0.08	0.04	0.06	0.06	0.06	0.06	0.06	0.06	0.06	15.7	19.2	8.6	13.1	14.1	0	0	1	1	0
DR−27Ts	0.541	0.53	0.53	0.54	0.52	0.53	0.03	0.03	0.00	0.03	0.02	0.07	0.07	0.08	0.07	0.07	4.9	5.5	0.3	6.7	4.2	1	1	1	1	1
DR−28ab	0.160	0.15	0.14	0.15	0.15	0.15	0.01	0.04	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	8.4	29.7	14.9	15.7	16.9	1	0	0	0	0
DR−25nor30ab	0.070	0.07	0.06	0.06	0.07	0.07	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	3.0	23.8	20.1	10.1	13.9	1	0	0	1	1
DR−29Ts	0.143	0.15	0.15	0.15	0.15	0.15	0.02	0.02	0.01	0.02	0.02	0.02	0.02	0.02	0.02	0.02	14.2	10.0	8.2	10.3	10.7	0	1	1	1	1
DR−30O	0.040	0.07	0.08	0.06	0.07	0.07	0.05	0.08	0.05	0.06	0.06	0.01	0.01	0.01	0.01	0.01	79.3	97.1	74.7	82.8	84.1	0	0	0	0	0
DR−30G	0.153	0.15	0.14	0.14	0.14	0.14	0.01	0.03	0.02	0.03	0.02	0.02	0.02	0.02	0.02	0.02	9.0	24.9	13.3	18.0	16.2	1	0	1	0	0
DR−29ab	0.856	0.88	0.90	0.86	0.89	0.88	0.05	0.09	0.01	0.07	0.05	0.12	0.13	0.12	0.12	0.12	5.2	9.7	1.4	8.0	6.1	1	1	1	1	1
DR−30d	0.050	0.05	0.05	0.05	0.05	0.05	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.01	8.5	17.5	15.5	12.4	8.7	1	0	0	1	1
DR−29aaS **m/z217**	0.984	0.93	0.94	0.92	0.95	0.93	0.11	0.09	0.12	0.07	0.10	0.13	0.13	0.13	0.13	0.13	12.2	10.1	13.0	7.2	10.6	1	1	1	1	1
DR−29bb **&218**	1.176	1.08	1.04	1.08	1.05	1.06	0.19	0.28	0.19	0.26	0.23	0.15	0.15	0.15	0.15	0.15	17.9	27.1	17.7	24.4	21.7	0	0	0	0	0
DR−27bbSTER	0.831	0.79	0.79	0.80	0.79	0.79	0.08	0.09	0.07	0.09	0.08	0.11	0.11	0.11	0.11	0.11	10.5	11.5	8.4	11.1	10.3	1	1	1	1	1
DR−28bbSTER	0.315	0.31	0.32	0.32	0.31	0.31	0.01	0.00	0.00	0.00	0.00	0.04	0.04	0.04	0.04	0.04	2.5	0.3	0.9	1.2	0.6	1	1	1	1	1
DR−29bbSTER	0.443	0.48	0.47	0.46	0.47	0.47	0.07	0.06	0.04	0.06	0.06	0.07	0.07	0.06	0.07	0.07	13.9	12.7	8.8	13.5	12.2	1	1	1	1	1
DR−TA21 **m/z231**	5.626	5.24	4.79	5.13	5.11	5.07	0.76	1.67	0.99	1.03	1.11	0.73	0.67	0.72	0.72	0.71	14.6	34.8	19.2	20.1	21.9	0	0	0	0	0
DR−TA26	0.533	0.49	0.51	0.49	0.48	0.49	0.09	0.05	0.09	0.10	0.08	0.07	0.07	0.07	0.07	0.07	18.8	9.9	19.2	21.5	17.2	0	1	0	0	0
DR−TA27	1.082	1.06	1.06	1.05	1.05	1.06	0.05	0.04	0.06	0.06	0.05	0.15	0.15	0.15	0.15	0.15	4.9	3.4	6.1	5.4	4.9	1	1	1	1	1
DR−2MP/1MP **PAH**	2.100	2.12	2.14	2.12	2.13	2.13	0.04	0.07	0.05	0.05	0.05	0.30	0.30	0.30	0.30	0.30	2.1	3.4	2.3	2.5	2.6	1	1	1	1	1
DR−4MD/1MD	2.353	2.39	2.41	2.38	2.40	2.40	0.08	0.11	0.06	0.09	0.09	0.34	0.34	0.33	0.34	0.34	3.4	4.5	2.5	3.8	3.6	1	1	1	1	1
DR−C2dbt/C2phe	0.523	0.57	0.59	0.57	0.58	0.58	0.10	0.14	0.09	0.11	0.11	0.08	0.08	0.08	0.08	0.08	17.8	23.9	15.2	18.7	19.0	0	0	0	0	0
DR−C3dbt/C3phe	0.642	0.72	0.74	0.70	0.71	0.72	0.15	0.19	0.12	0.14	0.15	0.10	0.10	0.10	0.10	0.10	21.4	26.0	17.6	20.0	21.3	0	0	0	0	0
DR−C3dbt/C3chr	2.288	2.62	2.83	2.45	2.56	2.61	0.66	1.08	0.33	0.55	0.65	0.37	0.40	0.34	0.36	0.37	25.2	38.1	13.4	21.6	25.0	0	0	1	0	0
DR−Retene/C4phe	0.053	0.05	0.05	0.05	0.05	0.05	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	16.8	17.7	20.2	15.8	17.6	0	0	0	0	0
DR−BaF/4Mpy	0.464	0.46	0.46	0.46	0.46	0.46	0.00	0.01	0.01	0.01	0.01	0.06	0.06	0.06	0.06	0.06	0.3	2.0	1.9	1.5	1.4	1	1	1	1	1
DR−BbcF/4Mpy	0.280	0.28	0.28	0.28	0.28	0.28	0.00	0.00	0.00	0.00	0.00	0.04	0.04	0.04	0.04	0.04	0.6	0.8	0.1	1.0	0.6	1	1	1	1	1
DR−2Mpy/4Mpy	0.970	0.96	0.96	0.96	0.97	0.97	0.02	0.01	0.02	0.01	0.01	0.13	0.14	0.13	0.14	0.14	1.7	1.1	1.6	0.8	0.9	1	1	1	1	1
DR−1Mpy/4Mpy	0.942	0.94	0.93	0.96	0.93	0.94	0.01	0.02	0.03	0.02	0.00	0.13	0.13	0.13	0.13	0.13	1.1	2.3	3.4	1.8	0.4	1	1	1	1	1
DR−SES1/SES2 **m/z123**	1.263	1.44	1.47	1.49	1.49	1.47	0.36	0.41	0.46	0.45	0.42	0.20	0.21	0.21	0.21	0.21	24.7	28.2	30.8	30.4	28.6	0	0	0	0	0
DR−SES3/SES5	0.235	0.35	0.31	0.32	0.33	0.33	0.22	0.15	0.17	0.18	0.18	0.05	0.04	0.04	0.05	0.05	64.2	49.2	52.6	55.3	55.6	0	0	0	0	0
DR−SES4/SES6	0.752	0.90	0.88	0.83	0.86	0.87	0.30	0.25	0.16	0.21	0.23	0.13	0.12	0.12	0.12	0.12	33.0	28.2	19.6	24.3	26.4	0	0	0	0	0
DR−SES5/SES10	0.478	0.69	0.73	0.71	0.71	0.71	0.42	0.51	0.46	0.46	0.46	0.10	0.10	0.10	0.10	0.10	60.9	69.2	64.5	65.1	65.0	0	0	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

	SINTEF ID	Test Date	Sample Description
1.	2007−0017	06−Feb−2007	Emulsion from ″TV−bukta″ by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2.	2007−0023	07−Feb−2007	Oil from shipwreck − "Server": Sample from Tank 3
3.	2007−0024	07−Feb−2007	Oil from shipwreck − "Server": Sample from Tank 4
4.	2007−0033	07−Feb−2007	Oil sample collected at KV ″ Eigun″

Figure E.10: Evaluation of diagnostic ratio (CEN Methods) of ″Server″ case of the oil spill sample (SINTEF ID: 2007-0018) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007–0282 Test Date: 07–May–2007 Description: Oil sample, Vetvika, Bremanger kommune, Nordfjord

Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR–C28 **m/z191**	0.222	0.22	0.22	0.23	0.23	0.22	0.00	0.01	0.02	0.01	0.00	0.03	0.03	0.03	0.03	0.03	0.8	6.4	7.3	5.2	1.5	1	1	1	1	1
DR–C29	0.179	0.17	0.17	0.18	0.17	0.17	0.01	0.02	0.00	0.02	0.01	0.02	0.02	0.02	0.02	0.02	8.6	9.3	2.7	10.5	7.7	1	1	1	1	1
DR–C28C29	0.402	0.39	0.39	0.41	0.40	0.40	0.02	0.03	0.01	0.01	0.01	0.06	0.05	0.06	0.06	0.06	4.2	7.7	2.9	1.5	2.5	1	1	1	1	1
DR–27Ts	0.485	0.50	0.50	0.51	0.50	0.50	0.03	0.03	0.06	0.02	0.03	0.07	0.07	0.07	0.07	0.07	6.1	5.6	11.3	4.4	6.9	1	1	1	1	1
DR–28ab	0.054	0.10	0.09	0.10	0.10	0.09	0.09	0.06	0.08	0.08	0.08	0.01	0.01	0.01	0.01	0.01	92.1	74.4	87.0	86.3	85.3	0	0	0	0	0
DR–25nor30ab	0.040	0.05	0.05	0.05	0.05	0.05	0.03	0.02	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.01	51.6	31.6	35.3	44.9	41.3	0	0	0	0	0
DR–29Ts	0.150	0.16	0.15	0.15	0.15	0.15	0.01	0.01	0.00	0.01	0.01	0.02	0.02	0.02	0.02	0.02	9.2	5.0	3.1	5.2	5.6	1	1	1	1	1
DR–30O	0.098	0.10	0.11	0.09	0.10	0.10	0.01	0.02	0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.01	6.0	16.1	11.4	1.8	0.2	1	0	1	1	1
DR–30G	0.130	0.13	0.12	0.13	0.13	0.13	0.01	0.01	0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.02	6.9	9.2	2.6	2.1	0.3	1	1	1	1	1
DR–29ab	0.873	0.89	0.91	0.87	0.90	0.89	0.03	0.07	0.00	0.05	0.04	0.12	0.13	0.12	0.13	0.12	3.3	7.8	0.5	6.1	4.2	1	1	1	1	1
DR–30d	0.044	0.05	0.04	0.04	0.04	0.04	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	22.1	3.8	1.8	1.3	5.1	0	1	1	1	1
DR–29aaS **m/z217**	0.970	0.92	0.93	0.92	0.94	0.93	0.10	0.08	0.11	0.05	0.09	0.13	0.13	0.13	0.13	0.13	10.8	8.7	11.6	5.8	9.2	1	1	1	1	1
DR–29bb **&218**	1.136	1.06	1.02	1.06	1.03	1.04	0.15	0.24	0.15	0.21	0.19	0.15	0.14	0.15	0.14	0.15	14.4	23.6	14.2	20.9	18.2	0	0	0	0	0
DR–27bbSTER	0.734	0.74	0.74	0.75	0.74	0.74	0.01	0.01	0.03	0.01	0.01	0.10	0.10	0.10	0.10	0.10	1.8	0.9	4.0	1.3	2.0	1	1	1	1	1
DR–28bbSTER	0.316	0.31	0.32	0.32	0.31	0.31	0.01	0.00	0.00	0.00	0.00	0.04	0.04	0.04	0.04	0.04	2.8	0.0	0.5	1.5	1.0	1	1	1	1	1
DR–29bbSTER	0.508	0.51	0.51	0.50	0.51	0.50	0.00	0.00	0.02	0.00	0.01	0.07	0.07	0.07	0.07	0.07	0.3	1.0	4.9	0.2	1.4	1	1	1	1	1
DR–TA21 **m/z231**	4.440	4.65	4.20	4.54	4.52	4.48	0.42	0.48	0.20	0.16	0.08	0.65	0.59	0.64	0.63	0.63	9.1	11.5	4.4	3.5	1.7	1	1	1	1	1
DR–TA26	0.424	0.43	0.45	0.43	0.43	0.44	0.02	0.06	0.02	0.01	0.02	0.06	0.06	0.06	0.06	0.06	4.0	13.0	3.6	1.3	5.6	1	1	1	1	1
DR–TA27	1.061	1.05	1.05	1.04	1.04	1.05	0.03	0.01	0.04	0.04	0.03	0.15	0.15	0.15	0.15	0.15	2.9	1.4	4.1	3.4	2.9	1	1	1	1	1
DR–2MP/1MP **PAH**	2.206	2.17	2.19	2.18	2.18	2.18	0.06	0.03	0.06	0.05	0.05	0.30	0.31	0.30	0.31	0.31	2.9	1.5	2.6	2.4	2.4	1	1	1	1	1
DR–4MD/1MD	2.469	2.45	2.47	2.44	2.46	2.45	0.03	0.01	0.06	0.02	0.03	0.34	0.35	0.34	0.34	0.34	1.4	0.3	2.3	1.0	1.3	1	1	1	1	1
DR–C2dbt/C2phe	0.655	0.64	0.66	0.63	0.64	0.64	0.03	0.01	0.05	0.02	0.02	0.09	0.09	0.09	0.09	0.09	4.5	1.6	7.1	3.7	3.4	1	1	1	1	1
DR–C3dbt/C3phe	0.780	0.79	0.81	0.77	0.78	0.79	0.02	0.05	0.01	0.00	0.02	0.11	0.11	0.11	0.11	0.11	2.0	6.7	1.8	0.6	1.9	1	1	1	1	1
DR–C3dbt/C3chr	2.426	2.69	2.90	2.52	2.63	2.68	0.52	0.94	0.19	0.41	0.52	0.38	0.41	0.35	0.37	0.38	19.4	32.4	7.5	15.7	19.2	0	0	1	0	0
DR–Retene/C4phe	0.045	0.04	0.04	0.04	0.04	0.04	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.5	0.4	3.0	1.5	0.4	1	1	1	1	1
DR–BaF/4Mpy	0.439	0.45	0.45	0.45	0.45	0.45	0.02	0.02	0.02	0.02	0.02	0.06	0.06	0.06	0.06	0.06	5.3	3.5	3.6	4.0	4.1	1	1	1	1	1
DR–BbcF/4Mpy	0.294	0.29	0.29	0.29	0.29	0.29	0.01	0.01	0.01	0.01	0.01	0.04	0.04	0.04	0.04	0.04	4.4	4.2	5.1	4.0	4.4	1	1	1	1	1
DR–2Mpy/4Mpy	0.967	0.96	0.96	0.96	0.97	0.96	0.01	0.01	0.01	0.01	0.01	0.13	0.13	0.13	0.14	0.13	1.3	0.8	1.3	1.1	0.6	1	1	1	1	1
DR–1Mpy/4Mpy	0.903	0.92	0.91	0.94	0.91	0.92	0.03	0.02	0.07	0.02	0.04	0.13	0.13	0.13	0.13	0.13	3.2	2.0	7.6	2.5	3.8	1	1	1	1	1
DR–SES1/SES2 **m/z123**	1.859	1.74	1.77	1.79	1.79	1.77	0.24	0.18	0.14	0.14	0.18	0.24	0.25	0.25	0.25	0.25	13.8	10.3	7.6	8.0	9.9	1	1	1	1	1
DR–SES3/SES5	1.273	0.87	0.83	0.84	0.84	0.84	0.82	0.88	0.87	0.86	0.86	0.12	0.12	0.12	0.12	0.12	94.2	106.4	103.8	101.7	101.5	0	0	0	0	0
DR–SES4/SES6	0.099	0.57	0.55	0.51	0.53	0.54	0.95	0.90	0.82	0.86	0.88	0.08	0.08	0.07	0.07	0.08	165.5	163.9	160.9	162.6	163.3	0	0	0	0	0
DR–SES5/SES10	0.266	0.58	0.62	0.60	0.60	0.60	0.63	0.72	0.67	0.67	0.67	0.08	0.09	0.08	0.08	0.08	108.5	114.9	111.3	111.8	111.7	0	0	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2007–0017	06–Feb–2007	Emulsion from "TV–bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2. 2007–0023	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 3
3. 2007–0024	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 4
4. 2007–0033	07–Feb–2007	Oil sample collected at KV " Eigun"

Figure E.11: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0282) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007-0019 Test Date: 07-Feb-2007 Description: Kelp from rullestein strand, Herdla vest.

Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR-C28 **m/z191**	0.224	0.22	0.22	0.23	0.23	0.22	0.00	0.02	0.02	0.01	0.00	0.03	0.03	0.03	0.03	0.03	1.5	7.1	6.6	4.5	0.8	1	1	1	1	1
DR-C29	0.172	0.17	0.17	0.17	0.17	0.17	0.01	0.01	0.00	0.01	0.01	0.02	0.02	0.02	0.02	0.02	4.6	5.3	1.2	6.5	3.7	1	1	1	1	1
DR-C28C29	0.396	0.39	0.38	0.40	0.40	0.39	0.01	0.02	0.02	0.00	0.00	0.05	0.05	0.06	0.06	0.06	2.8	6.3	4.3	0.1	1.2	1	1	1	1	1
DR-27Ts	0.545	0.53	0.53	0.54	0.53	0.53	0.03	0.03	0.00	0.04	0.03	0.07	0.07	0.08	0.07	0.07	5.5	6.1	0.3	7.2	4.7	1	1	1	1	1
DR-28ab	0.118	0.13	0.12	0.13	0.13	0.13	0.03	0.00	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	22.6	1.2	16.2	15.4	14.2	0	1	0	0	0
DR-25nor30ab	0.058	0.06	0.06	0.06	0.06	0.06	0.01	0.00	0.00	0.01	0.00	0.01	0.01	0.01	0.01	0.01	15.9	5.0	1.2	8.8	5.0	0	1	1	1	1
DR-29Ts	0.150	0.16	0.15	0.15	0.15	0.15	0.01	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.02	9.4	5.2	3.4	5.4	5.9	1	1	1	1	1
DR-30O	0.083	0.09	0.10	0.09	0.09	0.09	0.01	0.03	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	10.2	32.2	4.9	14.4	16.0	1	0	1	0	0
DR-30G	0.129	0.13	0.12	0.13	0.13	0.13	0.01	0.01	0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.02	8.0	8.0	3.7	1.0	0.8	1	1	1	1	1
DR-29ab	0.874	0.89	0.91	0.87	0.90	0.89	0.03	0.07	0.01	0.05	0.04	0.12	0.13	0.12	0.13	0.12	3.1	7.6	0.7	5.9	4.0	1	1	1	1	1
DR-30d	0.043	0.05	0.04	0.04	0.04	0.04	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	24.1	1.8	0.2	3.3	7.0	0	1	1	1	1
DR-29aaS **m/z217**	0.908	0.89	0.90	0.89	0.91	0.90	0.04	0.02	0.04	0.01	0.02	0.12	0.13	0.12	0.13	0.13	4.2	2.1	5.0	0.9	2.6	1	1	1	1	1
DR-29bb **&218**	0.975	0.98	0.94	0.98	0.95	0.96	0.01	0.08	0.01	0.05	0.03	0.14	0.13	0.14	0.13	0.13	0.8	8.5	1.0	5.7	3.0	1	1	1	1	1
DR-27bbSTER	0.741	0.74	0.74	0.75	0.74	0.75	0.01	0.00	0.02	0.00	0.01	0.10	0.10	0.11	0.10	0.10	0.9	0.1	3.1	0.4	1.1	1	1	1	1	1
DR-28bbSTER	0.324	0.32	0.32	0.32	0.32	0.32	0.02	0.01	0.01	0.01	0.01	0.04	0.04	0.04	0.04	0.04	5.5	2.7	2.2	4.2	3.6	1	1	1	1	1
DR-29bbSTER	0.491	0.50	0.50	0.49	0.50	0.50	0.02	0.01	0.01	0.02	0.01	0.07	0.07	0.07	0.07	0.07	3.5	2.3	1.6	3.1	1.8	1	1	1	1	1
DR-TA21 **m/z231**	4.822	4.84	4.39	4.73	4.71	4.67	0.04	0.86	0.18	0.22	0.31	0.68	0.61	0.66	0.66	0.65	0.8	19.7	3.8	4.7	6.6	1	0	1	1	1
DR-TA26	0.426	0.43	0.45	0.43	0.43	0.44	0.02	0.06	0.01	0.00	0.02	0.06	0.06	0.06	0.06	0.06	3.5	12.5	3.1	0.8	5.1	1	1	1	1	1
DR-TA27	1.069	1.05	1.06	1.04	1.05	1.05	0.04	0.02	0.05	0.04	0.04	0.15	0.15	0.15	0.15	0.15	3.7	2.2	4.9	4.2	3.7	1	1	1	1	1
DR-2MP/1MP **PAH**	2.143	2.14	2.16	2.15	2.15	2.15	0.00	0.03	0.01	0.01	0.01	0.30	0.30	0.30	0.30	0.30	0.0	1.4	0.3	0.5	0.5	1	1	1	1	1
DR-4MD/1MD	2.416	2.43	2.44	2.41	2.43	2.43	0.02	0.04	0.00	0.03	0.02	0.34	0.34	0.34	0.34	0.34	0.7	1.8	0.1	1.2	0.9	1	1	1	1	1
DR-C2dbt/C2phe	0.612	0.62	0.64	0.61	0.62	0.62	0.01	0.05	0.00	0.02	0.02	0.09	0.09	0.09	0.09	0.09	2.3	8.4	0.3	3.1	3.4	1	1	1	1	1
DR-C3dbt/C3phe	0.759	0.78	0.80	0.76	0.77	0.78	0.04	0.07	0.01	0.03	0.04	0.11	0.11	0.11	0.11	0.11	4.7	9.4	0.9	3.3	4.6	1	1	1	1	1
DR-C3dbt/C3chr	2.975	2.96	3.17	2.80	2.91	2.96	0.03	0.39	0.36	0.14	0.03	0.41	0.44	0.39	0.41	0.41	1.0	12.3	12.9	4.6	1.1	1	1	1	1	1
DR-Retene/C4phe	0.038	0.04	0.04	0.04	0.04	0.04	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	16.4	15.5	13.0	17.4	15.6	0	0	1	0	0
DR-BaF/4Mpy	0.457	0.46	0.46	0.46	0.46	0.46	0.01	0.00	0.00	0.00	0.00	0.06	0.06	0.06	0.06	0.06	1.2	0.5	0.4	0.0	0.1	1	1	1	1	1
DR-BbcF/4Mpy	0.266	0.27	0.27	0.27	0.27	0.27	0.02	0.02	0.01	0.02	0.02	0.04	0.04	0.04	0.04	0.04	5.7	5.9	4.9	6.1	5.6	1	1	1	1	1
DR-2Mpy/4Mpy	0.965	0.96	0.96	0.96	0.97	0.96	0.01	0.01	0.01	0.01	0.00	0.13	0.13	0.13	0.14	0.13	1.2	0.6	1.1	1.2	0.4	1	1	1	1	1
DR-1Mpy/4Mpy	0.922	0.93	0.92	0.95	0.92	0.93	0.01	0.00	0.05	0.00	0.02	0.13	0.13	0.13	0.13	0.13	1.1	0.1	5.6	0.4	1.8	1	1	1	1	1
DR-SES1/SES2 **m/z123**	1.611	1.61	1.64	1.67	1.66	1.65	0.01	0.07	0.11	0.10	0.07	0.23	0.23	0.23	0.23	0.23	0.5	4.0	6.7	6.3	4.4	1	1	1	1	1
DR-SES3/SES5	0.383	0.42	0.39	0.39	0.40	0.40	0.07	0.01	0.02	0.03	0.03	0.06	0.05	0.06	0.06	0.06	17.8	1.5	5.1	8.0	8.3	0	1	1	1	1
DR-SES4/SES6	0.980	1.01	0.99	0.95	0.97	0.98	0.07	0.02	0.06	0.02	0.00	0.14	0.14	0.13	0.14	0.14	6.8	1.9	6.8	2.0	0.1	1	1	1	1	1
DR-SES5/SES10	0.845	0.87	0.91	0.89	0.89	0.89	0.05	0.14	0.09	0.09	0.09	0.12	0.13	0.12	0.12	0.12	5.8	15.1	9.8	10.5	10.4	1	0	1	1	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

	SINTEF ID	**Test Date**	**Sample Description**
1.	2007-0017	06-Feb-2007	Emulsion from "TV-bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2.	2007-0023	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 3
3.	2007-0024	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 4
4.	2007-0033	07-Feb-2007	Oil sample collected at KV " Eigun"

Figure E.12: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0019) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007–0394 Test Date: 02–Aug–2007 Description: Oil sample (nr. 1), Fyrsundet position 2, Fedje

Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR–C28 **m/z191**	0.231	0.23	0.22	0.24	0.23	0.23	0.01	0.02	0.01	0.00	0.01	0.03	0.03	0.03	0.03	0.03	4.7	10.3	3.4	1.3	2.4	1	1	1	1	1
DR–C29	0.178	0.17	0.17	0.18	0.17	0.17	0.01	0.01	0.00	0.02	0.01	0.02	0.02	0.02	0.02	0.02	8.1	8.7	2.2	9.9	7.2	1	1	1	1	1
DR–C28C29	0.410	0.40	0.39	0.41	0.40	0.40	0.02	0.04	0.00	0.01	0.02	0.06	0.05	0.06	0.06	0.06	6.2	9.6	1.0	3.5	4.5	1	1	1	1	1
DR–27Ts	0.516	0.52	0.51	0.53	0.51	0.52	0.00	0.00	0.03	0.01	0.00	0.07	0.07	0.07	0.07	0.07	0.0	0.6	5.2	1.8	0.7	1	1	1	1	1
DR–28ab	0.106	0.13	0.11	0.12	0.12	0.12	0.04	0.01	0.03	0.03	0.03	0.02	0.02	0.02	0.02	0.02	32.7	11.5	26.4	25.6	24.4	0	1	0	0	0
DR–25nor30ab	0.040	0.05	0.05	0.05	0.05	0.05	0.03	0.02	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.01	52.4	32.4	36.1	45.7	42.1	0	0	0	0	0
DR–29Ts	0.161	0.16	0.16	0.16	0.16	0.16	0.00	0.00	0.01	0.00	0.00	0.02	0.02	0.02	0.02	0.02	2.2	2.0	3.8	1.8	1.3	1	1	1	1	1
DR–30O	0.094	0.09	0.10	0.09	0.10	0.10	0.00	0.02	0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.01	1.7	20.4	7.1	2.5	4.1	1	0	1	1	1
DR–30G	0.135	0.14	0.13	0.13	0.13	0.13	0.00	0.02	0.00	0.01	0.00	0.02	0.02	0.02	0.02	0.02	3.4	12.6	0.9	5.6	3.7	1	1	1	1	1
DR–29ab	0.914	0.91	0.93	0.89	0.92	0.91	0.01	0.03	0.05	0.01	0.00	0.13	0.13	0.12	0.13	0.13	1.4	3.1	5.2	1.4	0.5	1	1	1	1	1
DR–30d	0.041	0.05	0.04	0.04	0.04	0.04	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	27.4	1.5	3.6	6.7	10.4	0	1	1	1	1
DR–29aaS **m/z217**	0.941	0.91	0.92	0.90	0.93	0.91	0.07	0.05	0.08	0.03	0.06	0.13	0.13	0.13	0.13	0.13	7.8	5.6	8.6	2.7	6.2	1	1	1	1	1
DR–29bb **&218**	1.109	1.05	1.00	1.05	1.01	1.03	0.13	0.21	0.12	0.19	0.16	0.15	0.14	0.15	0.14	0.14	12.0	21.2	11.8	18.5	15.8	1	0	1	0	0
DR–27bbSTER	0.698	0.72	0.72	0.73	0.72	0.72	0.05	0.04	0.07	0.05	0.05	0.10	0.10	0.10	0.10	0.10	6.9	6.0	9.1	6.4	7.1	1	1	1	1	1
DR–28bbSTER	0.328	0.32	0.32	0.32	0.32	0.32	0.02	0.01	0.01	0.02	0.02	0.04	0.05	0.05	0.04	0.04	6.8	4.0	3.4	5.5	4.9	1	1	1	1	1
DR–29bbSTER	0.519	0.51	0.51	0.50	0.51	0.51	0.01	0.02	0.04	0.01	0.02	0.07	0.07	0.07	0.07	0.07	2.0	3.2	7.1	2.4	3.7	1	1	1	1	1
DR–TA21 **m/z231**	3.291	4.08	3.63	3.97	3.95	3.90	1.57	0.67	1.35	1.31	1.22	0.57	0.51	0.56	0.55	0.55	38.5	18.4	34.0	33.2	31.4	0	0	0	0	0
DR–TA26	0.420	0.43	0.45	0.43	0.42	0.43	0.02	0.06	0.02	0.01	0.03	0.06	0.06	0.06	0.06	0.06	4.9	13.9	4.5	2.2	6.5	1	1	1	1	1
DR–TA27	1.049	1.04	1.05	1.03	1.04	1.04	0.02	0.00	0.03	0.02	0.02	0.15	0.15	0.14	0.15	0.15	1.8	0.3	3.0	2.3	1.8	1	1	1	1	1
DR–2MP/1MP **PAH**	2.019	2.08	2.10	2.08	2.09	2.09	0.12	0.15	0.13	0.13	0.13	0.29	0.29	0.29	0.29	0.29	6.0	7.3	6.2	6.4	6.5	1	1	1	1	1
DR–4MD/1MD	2.397	2.42	2.43	2.41	2.42	2.42	0.04	0.06	0.02	0.05	0.04	0.34	0.34	0.34	0.34	0.34	1.5	2.6	0.7	1.9	1.7	1	1	1	1	1
DR–C2dbt/C2phe	0.664	0.64	0.66	0.64	0.65	0.65	0.04	0.00	0.05	0.03	0.03	0.09	0.09	0.09	0.09	0.09	5.9	0.2	8.5	5.0	4.7	1	1	1	1	1
DR–C3dbt/C3phe	0.817	0.81	0.83	0.79	0.80	0.81	0.02	0.02	0.05	0.03	0.02	0.11	0.12	0.11	0.11	0.11	2.7	2.1	6.5	4.0	2.7	1	1	1	1	1
DR–C3dbt/C3chr	2.455	2.70	2.91	2.54	2.65	2.70	0.49	0.91	0.16	0.39	0.49	0.38	0.41	0.35	0.37	0.38	18.2	31.3	6.3	14.5	18.0	0	0	1	0	0
DR–Retene/C4phe	0.044	0.04	0.04	0.04	0.04	0.04	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	2.0	1.1	1.4	3.0	1.2	1	1	1	1	1
DR–BaF/4Mpy	0.485	0.47	0.47	0.47	0.47	0.47	0.02	0.03	0.03	0.03	0.03	0.07	0.07	0.07	0.07	0.07	4.7	6.5	6.4	6.0	5.9	1	1	1	1	1
DR–BbcF/4Mpy	0.281	0.28	0.28	0.28	0.28	0.28	0.00	0.00	0.00	0.00	0.00	0.04	0.04	0.04	0.04	0.04	0.2	0.4	0.5	0.6	0.2	1	1	1	1	1
DR–2Mpy/4Mpy	0.999	0.98	0.98	0.98	0.99	0.98	0.04	0.04	0.04	0.02	0.04	0.14	0.14	0.14	0.14	0.14	4.6	4.0	4.5	2.1	3.8	1	1	1	1	1
DR–1Mpy/4Mpy	0.941	0.94	0.93	0.96	0.93	0.94	0.01	0.02	0.03	0.02	0.00	0.13	0.13	0.13	0.13	0.13	1.0	2.2	3.5	1.7	0.3	1	1	1	1	1
DR–SES1/SES2 **m/z123**	2.091	1.86	1.88	1.91	1.90	1.89	0.47	0.41	0.37	0.38	0.41	0.26	0.26	0.27	0.27	0.26	25.4	22.0	19.3	19.7	21.6	0	0	0	0	0
DR–SES3/SES5	0.447	0.45	0.42	0.43	0.43	0.43	0.01	0.06	0.04	0.03	0.03	0.06	0.06	0.06	0.06	0.06	2.3	14.0	10.4	7.5	7.2	1	0	1	1	1
DR–SES4/SES6	1.023	1.04	1.01	0.97	0.99	1.00	0.03	0.02	0.11	0.06	0.04	0.14	0.14	0.14	0.14	0.14	2.5	2.3	11.1	6.3	4.2	1	1	1	1	1
DR–SES5/SES10	0.819	0.86	0.90	0.88	0.88	0.88	0.08	0.16	0.11	0.12	0.12	0.12	0.13	0.12	0.12	0.12	8.9	18.2	12.9	13.6	13.5	1	0	1	1	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2007–0017	06–Feb–2007	Emulsion from "TV–bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2. 2007–0023	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 3
3. 2007–0024	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 4
4. 2007–0033	07–Feb–2007	Oil sample collected at KV " Eigun"

Figure E.13: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0394) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007-0021 Test Date: 15-Jan-2007 Description: Oil /Emulsion from lense, Gudbrandsøy

Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR-C28 **m/z191**	0.226	0.22	0.22	0.23	0.23	0.23	0.01	0.02	0.01	0.01	0.00	0.03	0.03	0.03	0.03	0.03	2.4	8.0	5.6	3.5	0.2	1	1	1	1	1
DR-C29	0.175	0.17	0.17	0.17	0.17	0.17	0.01	0.01	0.00	0.01	0.01	0.02	0.02	0.02	0.02	0.02	6.4	7.0	0.5	8.2	5.5	1	1	1	1	1
DR-C28C29	0.401	0.39	0.39	0.41	0.40	0.40	0.02	0.03	0.01	0.01	0.01	0.06	0.05	0.06	0.06	0.06	4.1	7.6	3.0	1.5	2.5	1	1	1	1	1
DR-27Ts	0.513	0.51	0.51	0.53	0.51	0.52	0.00	0.00	0.03	0.01	0.01	0.07	0.07	0.07	0.07	0.07	0.4	0.1	5.6	1.3	1.2	1	1	1	1	1
DR-28ab	0.128	0.14	0.12	0.13	0.13	0.13	0.02	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.02	14.0	7.4	7.6	6.8	5.5	0	1	1	1	1
DR-25nor30ab	0.058	0.06	0.06	0.06	0.06	0.06	0.01	0.00	0.00	0.01	0.00	0.01	0.01	0.01	0.01	0.01	16.2	4.7	0.9	9.1	5.3	0	1	1	1	1
DR-29Ts	0.151	0.16	0.15	0.15	0.15	0.15	0.01	0.01	0.00	0.01	0.01	0.02	0.02	0.02	0.02	0.02	8.3	4.1	2.3	4.4	4.8	1	1	1	1	1
DR-30O	0.088	0.09	0.10	0.09	0.09	0.09	0.00	0.03	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	4.7	26.7	0.7	8.9	10.5	1	0	1	1	1
DR-30G	0.137	0.14	0.13	0.14	0.13	0.13	0.00	0.02	0.00	0.01	0.01	0.02	0.02	0.02	0.02	0.02	2.1	13.9	2.2	6.9	5.1	1	1	1	1	1
DR-29ab	0.884	0.89	0.91	0.88	0.91	0.90	0.02	0.06	0.02	0.04	0.03	0.12	0.13	0.12	0.13	0.13	2.0	6.5	1.8	4.8	3.0	1	1	1	1	1
DR-30d	0.052	0.05	0.05	0.05	0.05	0.05	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	3.9	22.0	20.0	16.9	13.2	1	0	0	0	1
DR-29aaS **m/z217**	0.898	0.88	0.89	0.88	0.91	0.89	0.03	0.01	0.03	0.02	0.01	0.12	0.13	0.12	0.13	0.12	3.1	0.9	3.8	2.0	1.4	1	1	1	1	1
DR-29bb **&218**	0.902	0.94	0.90	0.94	0.91	0.92	0.08	0.01	0.08	0.02	0.04	0.13	0.13	0.13	0.13	0.13	8.6	0.7	8.8	2.1	4.8	1	1	1	1	1
DR-27bbSTER	0.770	0.76	0.76	0.77	0.76	0.76	0.02	0.03	0.01	0.03	0.02	0.11	0.11	0.11	0.11	0.11	2.9	3.8	0.7	3.4	2.7	1	1	1	1	1
DR-28bbSTER	0.312	0.31	0.31	0.31	0.31	0.31	0.01	0.00	0.00	0.00	0.00	0.04	0.04	0.04	0.04	0.04	1.8	1.0	1.6	0.5	0.1	1	1	1	1	1
DR-29bbSTER	0.486	0.50	0.49	0.48	0.50	0.49	0.02	0.02	0.00	0.02	0.01	0.07	0.07	0.07	0.07	0.07	4.6	3.4	0.5	4.2	2.9	1	1	1	1	1
DR-TA21 **m/z231**	4.810	4.84	4.38	4.73	4.71	4.66	0.05	0.85	0.17	0.21	0.29	0.68	0.61	0.66	0.66	0.65	1.1	19.4	3.6	4.5	6.3	1	0	1	1	1
DR-TA26	0.458	0.45	0.47	0.45	0.44	0.45	0.02	0.03	0.02	0.03	0.01	0.06	0.07	0.06	0.06	0.06	3.6	5.3	4.0	6.4	2.1	1	1	1	1	1
DR-TA27	1.073	1.05	1.06	1.05	1.05	1.05	0.04	0.03	0.05	0.05	0.04	0.15	0.15	0.15	0.15	0.15	4.0	2.5	5.2	4.5	4.1	1	1	1	1	1
DR-2MP/1MP **PAH**	2.141	2.14	2.16	2.14	2.15	2.15	0.00	0.03	0.01	0.01	0.01	0.30	0.30	0.30	0.30	0.30	0.1	1.5	0.4	0.6	0.6	1	1	1	1	1
DR-4MD/1MD	2.430	2.43	2.45	2.42	2.44	2.43	0.00	0.03	0.02	0.01	0.01	0.34	0.34	0.34	0.34	0.34	0.2	1.3	0.7	0.6	0.3	1	1	1	1	1
DR-C2dbt/C2phe	0.616	0.62	0.64	0.61	0.62	0.62	0.01	0.05	0.01	0.01	0.02	0.09	0.09	0.09	0.09	0.09	1.5	7.6	1.1	2.4	2.7	1	1	1	1	1
DR-C3dbt/C3phe	0.760	0.78	0.80	0.76	0.77	0.78	0.04	0.07	0.01	0.02	0.04	0.11	0.11	0.11	0.11	0.11	4.6	9.3	0.8	3.2	4.5	1	1	1	1	1
DR-C3dbt/C3chr	2.448	2.70	2.91	2.53	2.64	2.70	0.50	0.92	0.17	0.39	0.49	0.38	0.41	0.35	0.37	0.38	18.5	31.5	6.6	14.8	18.3	0	0	1	0	0
DR-Retene/C4phe	0.039	0.04	0.04	0.04	0.04	0.04	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	14.6	13.7	11.1	15.6	13.8	0	1	1	0	1
DR-BaF/4Mpy	0.455	0.46	0.45	0.46	0.46	0.46	0.01	0.00	0.00	0.00	0.00	0.06	0.06	0.06	0.06	0.06	1.7	0.1	0.0	0.4	0.5	1	1	1	1	1
DR-BbcF/4Mpy	0.271	0.28	0.28	0.28	0.28	0.28	0.01	0.01	0.01	0.01	0.01	0.04	0.04	0.04	0.04	0.04	3.7	3.9	3.0	4.1	3.7	1	1	1	1	1
DR-2Mpy/4Mpy	0.963	0.96	0.96	0.96	0.97	0.96	0.01	0.00	0.01	0.01	0.00	0.13	0.13	0.13	0.14	0.13	0.9	0.3	0.9	1.5	0.1	1	1	1	1	1
DR-1Mpy/4Mpy	0.976	0.95	0.95	0.98	0.95	0.96	0.04	0.05	0.00	0.05	0.04	0.13	0.13	0.14	0.13	0.13	4.6	5.8	0.1	5.3	3.9	1	1	1	1	1
DR-SES1/SES2 **m/z123**	1.596	1.61	1.64	1.66	1.66	1.64	0.02	0.08	0.13	0.12	0.09	0.23	0.23	0.23	0.23	0.23	1.4	5.0	7.7	7.2	5.4	1	1	1	1	1
DR-SES3/SES5	0.365	0.41	0.38	0.38	0.39	0.39	0.09	0.02	0.04	0.05	0.05	0.06	0.05	0.05	0.05	0.05	22.5	6.3	9.9	12.8	13.1	0	1	1	1	1
DR-SES4/SES6	0.915	0.98	0.96	0.92	0.94	0.95	0.13	0.08	0.00	0.04	0.07	0.14	0.13	0.13	0.13	0.13	13.6	8.7	0.0	4.8	6.9	1	1	1	1	1
DR-SES5/SES10	0.869	0.88	0.93	0.90	0.90	0.90	0.03	0.11	0.06	0.07	0.07	0.12	0.13	0.13	0.13	0.13	3.0	12.3	7.1	7.7	7.6	1	1	1	1	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

	SINTEF ID	**Test Date**	**Sample Description**
1.	2007-0017	06-Feb-2007	Emulsion from "TV-bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2.	2007-0023	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 3
3.	2007-0024	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 4
4.	2007-0033	07-Feb-2007	Oil sample collected at KV " Eigun"

Figure E.14: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0021) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007–0063 Test Date: 08–Feb–2007 Description: Oil sample, Kvamsøy, Sande Kommune,

Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR–C28 **m/z191**	0.205	0.21	0.21	0.22	0.22	0.22	0.02	0.00	0.03	0.03	0.02	0.03	0.03	0.03	0.03	0.03	7.4	1.8	15.5	13.4	9.7	1	1	0	1	1
DR–C29	0.157	0.16	0.16	0.17	0.16	0.16	0.01	0.01	0.02	0.00	0.01	0.02	0.02	0.02	0.02	0.02	4.8	4.2	10.7	3.0	5.7	1	1	1	1	1
DR–C28C29	0.362	0.37	0.37	0.39	0.38	0.38	0.02	0.01	0.05	0.03	0.03	0.05	0.05	0.05	0.05	0.05	6.3	2.8	13.4	9.0	8.0	1	1	1	1	1
DR–27Ts	0.506	0.51	0.51	0.52	0.51	0.51	0.01	0.01	0.04	0.00	0.01	0.07	0.07	0.07	0.07	0.07	1.8	1.2	7.0	0.0	2.5	1	1	1	1	1
DR–28ab	0.107	0.13	0.11	0.12	0.12	0.12	0.04	0.01	0.03	0.03	0.03	0.02	0.02	0.02	0.02	0.02	31.8	10.5	25.4	24.7	23.4	0	1	0	0	0
DR–25nor30ab	0.041	0.05	0.05	0.05	0.05	0.05	0.03	0.01	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.01	49.9	29.9	33.5	43.2	39.5	0	0	0	0	0
DR–29Ts	0.155	0.16	0.16	0.15	0.16	0.16	0.01	0.00	0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.02	6.1	1.8	0.0	2.1	2.5	1	1	1	1	1
DR–30O	0.094	0.09	0.10	0.09	0.10	0.10	0.00	0.02	0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.01	1.8	20.4	7.1	2.5	4.0	1	0	1	1	1
DR–30G	0.128	0.13	0.12	0.13	0.13	0.13	0.01	0.01	0.01	0.00	0.00	0.02	0.02	0.02	0.02	0.02	8.7	7.3	4.4	0.3	1.6	1	1	1	1	1
DR–29ab	0.871	0.89	0.91	0.87	0.90	0.89	0.03	0.07	0.00	0.06	0.04	0.12	0.13	0.12	0.13	0.12	3.5	8.0	0.3	6.3	4.4	1	1	1	1	1
DR–30d	0.046	0.05	0.04	0.04	0.05	0.05	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	16.6	9.4	7.4	4.3	0.5	0	1	1	1	1
DR–29aaS **m/z217**	0.978	0.92	0.93	0.92	0.95	0.93	0.11	0.09	0.11	0.06	0.09	0.13	0.13	0.13	0.13	0.13	11.6	9.4	12.3	6.5	9.9	1	1	1	1	1
DR–29bb **&218**	0.923	0.95	0.91	0.95	0.92	0.93	0.06	0.03	0.06	0.00	0.02	0.13	0.13	0.13	0.13	0.13	6.3	3.0	6.5	0.2	2.5	1	1	1	1	1
DR–27bbSTER	0.735	0.74	0.74	0.75	0.74	0.74	0.01	0.01	0.03	0.01	0.01	0.10	0.10	0.10	0.10	0.10	1.8	0.8	3.9	1.2	1.9	1	1	1	1	1
DR–28bbSTER	0.311	0.31	0.31	0.31	0.31	0.31	0.00	0.00	0.01	0.00	0.00	0.04	0.04	0.04	0.04	0.04	1.4	1.4	1.9	0.1	0.4	1	1	1	1	1
DR–29bbSTER	0.513	0.51	0.51	0.50	0.51	0.51	0.00	0.01	0.03	0.01	0.01	0.07	0.07	0.07	0.07	0.07	0.8	2.0	5.9	1.2	2.4	1	1	1	1	1
DR–TA21 **m/z231**	3.997	4.43	3.98	4.32	4.30	4.26	0.86	0.04	0.64	0.60	0.52	0.62	0.56	0.60	0.60	0.60	19.5	1.0	14.9	14.0	12.2	0	1	0	0	1
DR–TA26	0.438	0.44	0.46	0.44	0.43	0.44	0.00	0.05	0.00	0.01	0.01	0.06	0.06	0.06	0.06	0.06	0.9	9.9	0.5	1.8	2.5	1	1	1	1	1
DR–TA27	1.022	1.03	1.03	1.02	1.02	1.03	0.01	0.02	0.00	0.00	0.01	0.14	0.14	0.14	0.14	0.14	0.9	2.4	0.3	0.3	0.8	1	1	1	1	1
DR–2MP/1MP **PAH**	2.174	2.16	2.17	2.16	2.16	2.16	0.03	0.00	0.03	0.02	0.02	0.30	0.30	0.30	0.30	0.30	1.4	0.1	1.2	1.0	0.9	1	1	1	1	1
DR–4MD/1MD	2.435	2.43	2.45	2.42	2.44	2.44	0.00	0.03	0.02	0.01	0.00	0.34	0.34	0.34	0.34	0.34	0.0	1.1	0.9	0.4	0.1	1	1	1	1	1
DR–C2dbt/C2phe	0.636	0.63	0.65	0.62	0.63	0.63	0.01	0.03	0.03	0.00	0.00	0.09	0.09	0.09	0.09	0.09	1.6	4.5	4.2	0.8	0.5	1	1	1	1	1
DR–C3dbt/C3phe	0.772	0.78	0.80	0.77	0.78	0.78	0.02	0.06	0.01	0.01	0.02	0.11	0.11	0.11	0.11	0.11	2.9	7.7	0.9	1.6	2.9	1	1	1	1	1
DR–C3dbt/C3chr	2.673	2.81	3.02	2.64	2.76	2.81	0.27	0.69	0.06	0.17	0.27	0.39	0.42	0.37	0.39	0.39	9.7	22.9	2.2	6.1	9.6	1	0	1	1	1
DR–Retene/C4phe	0.028	0.04	0.04	0.04	0.04	0.04	0.02	0.02	0.02	0.02	0.02	0.01	0.01	0.00	0.01	0.01	46.2	45.3	42.9	47.1	45.4	0	0	0	0	0
DR–BaF/4Mpy	0.464	0.46	0.46	0.46	0.46	0.46	0.00	0.01	0.01	0.01	0.01	0.06	0.06	0.06	0.06	0.06	0.3	2.1	2.0	1.6	1.5	1	1	1	1	1
DR–BbcF/4Mpy	0.276	0.28	0.28	0.28	0.28	0.28	0.01	0.01	0.00	0.01	0.01	0.04	0.04	0.04	0.04	0.04	2.1	2.3	1.4	2.5	2.1	1	1	1	1	1
DR–2Mpy/4Mpy	0.970	0.96	0.96	0.96	0.97	0.97	0.02	0.01	0.02	0.01	0.01	0.13	0.14	0.13	0.14	0.14	1.7	1.1	1.6	0.8	0.9	1	1	1	1	1
DR–1Mpy/4Mpy	0.926	0.93	0.92	0.95	0.93	0.93	0.01	0.00	0.05	0.00	0.01	0.13	0.13	0.13	0.13	0.13	0.7	0.5	5.1	0.0	1.3	1	1	1	1	1
DR–SES1/SES2 **m/z123**	1.616	1.62	1.65	1.67	1.67	1.65	0.00	0.06	0.11	0.10	0.07	0.23	0.23	0.23	0.23	0.23	0.2	3.7	6.4	6.0	4.1	1	1	1	1	1
DR–SES3/SES5	0.397	0.43	0.39	0.40	0.41	0.41	0.06	0.01	0.01	0.02	0.02	0.06	0.05	0.06	0.06	0.06	14.3	2.0	1.6	4.5	4.8	0	1	1	1	1
DR–SES4/SES6	0.999	1.02	1.00	0.96	0.98	0.99	0.05	0.00	0.08	0.04	0.02	0.14	0.14	0.13	0.14	0.14	4.8	0.0	8.8	4.0	1.9	1	1	1	1	1
DR–SES5/SES10	0.883	0.89	0.93	0.91	0.91	0.91	0.01	0.10	0.05	0.06	0.05	0.12	0.13	0.13	0.13	0.13	1.4	10.7	5.5	6.1	6.0	1	1	1	1	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

	SINTEF ID	**Test Date**	**Sample Description**
1.	2007–0017	06–Feb–2007	Emulsion from "TV–bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2.	2007–0023	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 3
3.	2007–0024	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 4
4.	2007–0033	07–Feb–2007	Oil sample collected at KV " Eigun"

Figure E.15: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0063) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007-0395 Test Date: 02-Aug-2007 Description: Oil sample (nr. 2), Fyrsundet position 2, Fedje

Ratio Name		Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
			R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR-C28	m/z191	0.228	0.22	0.22	0.23	0.23	0.23	0.01	0.02	0.01	0.01	0.00	0.03	0.03	0.03	0.03	0.03	3.1	8.7	5.0	2.9	0.9	1	1	1	1	1
DR-C29		0.179	0.17	0.17	0.18	0.17	0.17	0.01	0.02	0.00	0.02	0.01	0.02	0.02	0.02	0.02	0.02	8.5	9.1	2.6	10.4	7.6	1	1	1	1	1
DR-C28C29		0.407	0.40	0.39	0.41	0.40	0.40	0.02	0.03	0.01	0.01	0.02	0.06	0.05	0.06	0.06	0.06	5.4	8.9	1.7	2.8	3.8	1	1	1	1	1
DR-27Ts		0.545	0.53	0.53	0.54	0.53	0.53	0.03	0.03	0.00	0.04	0.03	0.07	0.07	0.08	0.07	0.07	5.6	6.1	0.4	7.3	4.8	1	1	1	1	1
DR-28ab		0.098	0.12	0.11	0.12	0.12	0.12	0.05	0.02	0.04	0.04	0.04	0.02	0.02	0.02	0.02	0.02	40.1	19.1	33.8	33.1	31.9	0	0	0	0	0
DR-25nor30ab		0.063	0.07	0.06	0.06	0.06	0.06	0.01	0.01	0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.01	8.8	12.1	8.4	1.7	2.2	1	1	1	1	1
DR-29Ts		0.158	0.16	0.16	0.16	0.16	0.16	0.01	0.00	0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.02	4.3	0.1	1.8	0.3	0.8	1	1	1	1	1
DR-30O		0.097	0.09	0.11	0.09	0.10	0.10	0.00	0.02	0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.01	4.6	17.6	10.0	0.4	1.2	1	0	1	1	1
DR-30G		0.138	0.14	0.13	0.14	0.13	0.13	0.00	0.02	0.00	0.01	0.01	0.02	0.02	0.02	0.02	0.02	0.9	15.1	3.4	8.1	6.3	1	0	1	1	1
DR-29ab		0.962	0.93	0.95	0.92	0.94	0.94	0.06	0.02	0.09	0.04	0.05	0.13	0.13	0.13	0.13	0.13	6.5	2.0	10.3	3.7	5.6	1	1	1	1	1
DR-30d		0.046	0.05	0.04	0.04	0.04	0.05	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	17.6	8.4	6.4	3.3	0.5	0	1	1	1	1
DR-29aaS	m/z217	0.912	0.89	0.90	0.89	0.91	0.90	0.04	0.02	0.05	0.00	0.03	0.12	0.13	0.12	0.13	0.13	4.6	2.5	5.4	0.4	3.0	1	1	1	1	1
DR-29bb	&218	1.144	1.06	1.02	1.06	1.03	1.04	0.16	0.25	0.16	0.22	0.20	0.15	0.14	0.15	0.14	0.15	15.1	24.3	15.0	21.6	18.9	0	0	0	0	0
DR-27bbSTER		0.726	0.74	0.73	0.74	0.73	0.74	0.02	0.02	0.04	0.02	0.02	0.10	0.10	0.10	0.10	0.10	3.0	2.1	5.2	2.5	3.2	1	1	1	1	1
DR-28bbSTER		0.305	0.31	0.31	0.31	0.31	0.31	0.00	0.01	0.01	0.01	0.01	0.04	0.04	0.04	0.04	0.04	0.6	3.4	3.9	1.9	2.5	1	1	1	1	1
DR-29bbSTER		0.529	0.52	0.52	0.51	0.52	0.51	0.02	0.03	0.05	0.02	0.03	0.07	0.07	0.07	0.07	0.07	3.8	5.0	8.9	4.2	5.5	1	1	1	1	1
DR-TA21	m/z231	3.711	4.29	3.83	4.18	4.16	4.11	1.15	0.25	0.93	0.89	0.80	0.60	0.54	0.58	0.58	0.58	26.9	6.5	22.3	21.4	19.6	0	1	0	0	0
DR-TA26		0.345	0.39	0.41	0.39	0.39	0.40	0.10	0.14	0.09	0.08	0.10	0.06	0.06	0.05	0.05	0.06	24.5	33.3	24.2	21.8	26.1	0	0	0	0	0
DR-TA27		1.122	1.08	1.08	1.07	1.07	1.08	0.09	0.08	0.10	0.10	0.09	0.15	0.15	0.15	0.15	0.15	8.4	6.9	9.6	9.0	8.5	1	1	1	1	1
DR-2MP/1MP	PAH	2.142	2.14	2.16	2.15	2.15	2.15	0.00	0.03	0.01	0.01	0.01	0.30	0.30	0.30	0.30	0.30	0.1	1.4	0.3	0.5	0.6	1	1	1	1	1
DR-4MD/1MD		2.330	2.38	2.40	2.37	2.39	2.38	0.10	0.13	0.08	0.11	0.11	0.33	0.34	0.33	0.33	0.33	4.4	5.5	3.5	4.8	4.5	1	1	1	1	1
DR-C2dbt/C2phe		0.697	0.66	0.68	0.65	0.66	0.66	0.07	0.03	0.09	0.07	0.06	0.09	0.10	0.09	0.09	0.09	10.8	4.7	13.4	9.9	9.6	1	1	1	1	1
DR-C3dbt/C3phe		0.858	0.83	0.85	0.81	0.82	0.83	0.06	0.02	0.09	0.07	0.06	0.12	0.12	0.11	0.12	0.12	7.6	2.8	11.4	8.9	7.6	1	1	1	1	1
DR-C3dbt/C3chr		2.791	2.87	3.08	2.70	2.82	2.87	0.16	0.57	0.17	0.05	0.15	0.40	0.43	0.38	0.39	0.40	5.4	18.6	6.5	1.8	5.3	1	0	1	1	1
DR-Retene/C4phe		0.045	0.04	0.04	0.04	0.04	0.04	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.2	0.7	3.2	1.2	0.6	1	1	1	1	1
DR-BaF/4Mpy		0.433	0.45	0.44	0.44	0.44	0.45	0.03	0.02	0.02	0.02	0.02	0.06	0.06	0.06	0.06	0.06	6.7	4.9	5.0	5.4	5.5	1	1	1	1	1
DR-BbcF/4Mpy		0.254	0.27	0.27	0.27	0.27	0.27	0.03	0.03	0.03	0.03	0.03	0.04	0.04	0.04	0.04	0.04	10.3	10.5	9.5	10.7	10.2	1	1	1	1	1
DR-2Mpy/4Mpy		0.968	0.96	0.96	0.96	0.97	0.96	0.01	0.01	0.01	0.01	0.01	0.13	0.13	0.13	0.14	0.14	1.4	0.9	1.4	1.0	0.7	1	1	1	1	1
DR-1Mpy/4Mpy		0.912	0.92	0.92	0.94	0.92	0.92	0.02	0.01	0.06	0.01	0.03	0.13	0.13	0.13	0.13	0.13	2.2	1.0	6.7	1.6	2.9	1	1	1	1	1
DR-SES1/SES2	m/z123	1.744	1.68	1.71	1.73	1.73	1.71	0.12	0.07	0.02	0.03	0.06	0.24	0.24	0.24	0.24	0.24	7.4	3.9	1.2	1.6	3.5	1	1	1	1	1
DR-SES3/SES5		0.403	0.43	0.40	0.40	0.41	0.41	0.05	0.01	0.00	0.01	0.01	0.06	0.06	0.06	0.06	0.06	12.7	3.7	0.0	2.9	3.2	1	1	1	1	1
DR-SES4/SES6		0.992	1.02	1.00	0.95	0.98	0.99	0.06	0.01	0.08	0.03	0.01	0.14	0.14	0.13	0.14	0.14	5.6	0.7	8.0	3.3	1.1	1	1	1	1	1
DR-SES5/SES10		0.646	0.77	0.81	0.79	0.79	0.79	0.25	0.34	0.29	0.29	0.29	0.11	0.11	0.11	0.11	0.11	32.3	41.3	36.2	36.9	36.7	0	0	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

	SINTEF ID	Test Date	Sample Description
1.	2007-0017	06-Feb-2007	Emulsion from "TV-bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2.	2007-0023	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 3
3.	2007-0024	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 4
4.	2007-0033	07-Feb-2007	Oil sample collected at KV " Eigun"

Figure E.16: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0395) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007–0022 Test Date: 06–Feb–2007 Description: Oil from shipwreck – "Server": Sample from Tank 2

Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR–C28 **m/z191**	0.180	0.20	0.19	0.21	0.21	0.20	0.04	0.03	0.06	0.05	0.05	0.03	0.03	0.03	0.03	0.03	20.4	14.8	28.4	26.3	22.6	0	0	0	0	0
DR–C29	0.148	0.16	0.16	0.16	0.15	0.16	0.02	0.02	0.03	0.01	0.02	0.02	0.02	0.02	0.02	0.02	10.8	10.1	16.6	8.9	11.7	1	1	0	1	1
DR–C28C29	0.327	0.36	0.35	0.37	0.36	0.36	0.06	0.04	0.09	0.07	0.06	0.05	0.05	0.05	0.05	0.05	16.2	12.8	23.3	18.9	17.8	0	1	0	0	0
DR–27Ts	0.714	0.61	0.61	0.63	0.61	0.62	0.20	0.20	0.17	0.21	0.19	0.09	0.09	0.09	0.09	0.09	32.3	32.9	27.3	34.0	31.6	0	0	0	0	0
DR–28ab	0.109	0.13	0.11	0.12	0.12	0.12	0.04	0.01	0.03	0.03	0.03	0.02	0.02	0.02	0.02	0.02	30.4	9.1	24.0	23.3	22.0	0	1	0	0	0
DR–25nor30ab	0.068	0.07	0.06	0.06	0.07	0.06	0.00	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.9	19.9	16.2	6.2	10.0	1	0	0	1	1
DR–29Ts	0.176	0.17	0.17	0.17	0.17	0.17	0.01	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	6.8	11.0	12.8	10.8	10.3	1	1	1	1	1
DR–30O	0.364	0.23	0.24	0.23	0.23	0.23	0.27	0.25	0.28	0.27	0.27	0.03	0.03	0.03	0.03	0.03	119.0	103.7	122.5	116.3	115.2	0	0	0	0	0
DR–30G	0.105	0.12	0.11	0.12	0.12	0.12	0.03	0.01	0.03	0.02	0.02	0.02	0.02	0.02	0.02	0.02	27.9	12.0	23.6	19.0	20.8	0	1	0	0	0
DR–29ab	0.862	0.88	0.90	0.87	0.89	0.89	0.04	0.08	0.01	0.07	0.05	0.12	0.13	0.12	0.13	0.12	4.5	9.0	0.7	7.3	5.4	1	1	1	1	1
DR–30d	0.050	0.05	0.05	0.05	0.05	0.05	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.01	8.3	17.6	15.6	12.5	8.8	1	0	0	1	1
DR–29aaS **m/z217**	0.949	0.91	0.92	0.91	0.93	0.92	0.08	0.06	0.08	0.03	0.06	0.13	0.13	0.13	0.13	0.13	8.5	6.4	9.3	3.5	6.9	1	1	1	1	1
DR–29bb **&218**	0.923	0.95	0.91	0.95	0.92	0.93	0.06	0.03	0.06	0.00	0.02	0.13	0.13	0.13	0.13	0.13	6.3	3.0	6.5	0.2	2.5	1	1	1	1	1
DR–27bbSTER	0.701	0.72	0.72	0.73	0.72	0.73	0.05	0.04	0.06	0.04	0.05	0.10	0.10	0.10	0.10	0.10	6.4	5.5	8.6	5.9	6.6	1	1	1	1	1
DR–28bbSTER	0.332	0.32	0.32	0.32	0.32	0.32	0.03	0.02	0.01	0.02	0.02	0.04	0.05	0.05	0.04	0.05	7.9	5.1	4.5	6.6	6.0	1	1	1	1	1
DR–29bbSTER	0.512	0.51	0.51	0.50	0.51	0.51	0.00	0.01	0.03	0.01	0.01	0.07	0.07	0.07	0.07	0.07	0.6	1.8	5.7	1.0	2.2	1	1	1	1	1
DR–TA21 **m/z231**	3.170	4.02	3.56	3.91	3.88	3.84	1.69	0.79	1.47	1.43	1.35	0.56	0.50	0.55	0.54	0.54	42.1	22.1	37.7	36.8	35.0	0	0	0	0	0
DR–TA26	0.206	0.32	0.34	0.32	0.32	0.33	0.24	0.28	0.23	0.22	0.24	0.05	0.05	0.05	0.04	0.05	72.7	80.4	72.4	70.3	74.0	0	0	0	0	0
DR–TA27	1.075	1.05	1.06	1.05	1.05	1.05	0.04	0.03	0.06	0.05	0.04	0.15	0.15	0.15	0.15	0.15	4.2	2.7	5.4	4.7	4.2	1	1	1	1	1
DR–2MP/1MP **PAH**	2.089	2.12	2.13	2.12	2.12	2.12	0.05	0.08	0.06	0.06	0.07	0.30	0.30	0.30	0.30	0.30	2.6	3.9	2.8	3.0	3.1	1	1	1	1	1
DR–4MD/1MD	2.302	2.37	2.38	2.36	2.37	2.37	0.13	0.16	0.11	0.14	0.14	0.33	0.33	0.33	0.33	0.33	5.6	6.7	4.7	6.0	5.7	1	1	1	1	1
DR–C2dbt/C2phe	0.586	0.61	0.63	0.60	0.61	0.61	0.04	0.08	0.02	0.04	0.05	0.08	0.09	0.08	0.09	0.09	6.6	12.7	3.9	7.4	7.7	1	1	1	1	1
DR–C3dbt/C3phe	0.731	0.76	0.78	0.75	0.76	0.76	0.06	0.10	0.04	0.05	0.06	0.11	0.11	0.10	0.11	0.11	8.5	13.2	4.7	7.2	8.5	1	1	1	1	1
DR–C3dbt/C3chr	2.124	2.54	2.74	2.37	2.48	2.53	0.82	1.24	0.49	0.72	0.82	0.35	0.38	0.33	0.35	0.35	32.4	45.2	20.7	28.8	32.3	0	0	0	0	0
DR–Retene/C4phe	0.043	0.04	0.04	0.04	0.04	0.04	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	3.2	2.2	0.3	4.1	2.3	1	1	1	1	1
DR–BaF/4Mpy	0.466	0.46	0.46	0.46	0.46	0.46	0.00	0.01	0.01	0.01	0.01	0.07	0.06	0.06	0.06	0.06	0.7	2.5	2.4	2.0	1.9	1	1	1	1	1
DR–BbcF/4Mpy	0.297	0.29	0.29	0.29	0.29	0.29	0.02	0.02	0.02	0.01	0.02	0.04	0.04	0.04	0.04	0.04	5.5	5.3	6.2	5.1	5.5	1	1	1	1	1
DR–2Mpy/4Mpy	0.905	0.93	0.93	0.93	0.94	0.93	0.05	0.05	0.05	0.07	0.06	0.13	0.13	0.13	0.13	0.13	5.2	5.8	5.3	7.7	6.0	1	1	1	1	1
DR–1Mpy/4Mpy	0.914	0.92	0.92	0.94	0.92	0.93	0.02	0.01	0.06	0.01	0.02	0.13	0.13	0.13	0.13	0.13	2.0	0.8	6.4	1.3	2.6	1	1	1	1	1
DR–SES1/SES2 **m/z123**	1.572	1.60	1.62	1.65	1.64	1.63	0.05	0.11	0.15	0.14	0.11	0.22	0.23	0.23	0.23	0.23	3.0	6.5	9.2	8.8	6.9	1	1	1	1	1
DR–SES3/SES5	0.480	0.47	0.43	0.44	0.45	0.45	0.02	0.09	0.08	0.07	0.06	0.07	0.06	0.06	0.06	0.06	4.8	21.1	17.5	14.6	14.3	1	0	0	0	0
DR–SES4/SES6	1.104	1.08	1.05	1.01	1.03	1.04	0.06	0.11	0.19	0.14	0.12	0.15	0.15	0.14	0.14	0.15	5.2	10.0	18.7	14.0	11.8	1	1	0	1	1
DR–SES5/SES10	1.038	0.97	1.01	0.99	0.99	0.99	0.14	0.05	0.10	0.10	0.10	0.14	0.14	0.14	0.14	0.14	14.7	5.4	10.7	10.0	10.1	0	1	1	1	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

	SINTEF ID	Test Date	Sample Description
1.	2007–0017	06–Feb–2007	Emulsion from "TV–bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2.	2007–0023	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 3
3.	2007–0024	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 4
4.	2007–0033	07–Feb–2007	Oil sample collected at KV " Eigun"

Figure E.17: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0022) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007-0064 Test Date: 08-Feb-2007 Description: Oil sample, Kvamsøy, Sande Kommune,

Ratio Name		Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
			R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR-C28	**m/z191**	0.219	0.22	0.21	0.23	0.23	0.22	0.00	0.01	0.02	0.01	0.01	0.03	0.03	0.03	0.03	0.03	0.5	5.1	8.6	6.5	2.8	1	1	1	1	1
DR-C29		0.170	0.17	0.17	0.17	0.17	0.17	0.01	0.01	0.00	0.01	0.00	0.02	0.02	0.02	0.02	0.02	3.3	3.9	2.6	5.1	2.4	1	1	1	1	1
DR-C28C29		0.389	0.39	0.38	0.40	0.39	0.39	0.00	0.02	0.02	0.01	0.00	0.05	0.05	0.06	0.05	0.05	1.1	4.6	6.0	1.6	0.6	1	1	1	1	1
DR-27Ts		0.536	0.53	0.52	0.54	0.52	0.53	0.02	0.02	0.01	0.03	0.02	0.07	0.07	0.08	0.07	0.07	3.9	4.4	1.3	5.6	3.1	1	1	1	1	1
DR-28ab		0.120	0.13	0.12	0.13	0.13	0.13	0.03	0.00	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	20.7	0.7	14.3	13.5	12.3	0	1	0	1	1
DR-25nor30ab		0.037	0.05	0.05	0.05	0.05	0.05	0.03	0.02	0.02	0.03	0.02	0.01	0.01	0.01	0.01	0.01	59.8	40.2	43.8	53.3	49.7	0	0	0	0	0
DR-29Ts		0.158	0.16	0.16	0.16	0.16	0.16	0.01	0.00	0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.02	3.9	0.3	2.2	0.1	0.3	1	1	1	1	1
DR-30O		0.093	0.09	0.10	0.09	0.09	0.10	0.00	0.02	0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.01	1.0	21.2	6.3	3.3	4.8	1	0	1	1	1
DR-30G		0.135	0.14	0.13	0.13	0.13	0.13	0.00	0.02	0.00	0.01	0.00	0.02	0.02	0.02	0.02	0.02	3.5	12.5	0.8	5.5	3.7	1	1	1	1	1
DR-29ab		0.945	0.92	0.94	0.91	0.94	0.93	0.04	0.00	0.08	0.02	0.04	0.13	0.13	0.13	0.13	0.13	4.7	0.2	8.5	1.9	3.8	1	1	1	1	1
DR-30d		0.047	0.05	0.04	0.04	0.05	0.05	0.01	0.01	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	14.4	11.5	9.5	6.4	2.7	0	1	1	1	1
DR-29aaS	**m/z217**	0.932	0.90	0.91	0.90	0.92	0.91	0.06	0.04	0.07	0.02	0.05	0.13	0.13	0.13	0.13	0.13	6.8	4.6	7.6	1.7	5.1	1	1	1	1	1
DR-29bb	**&218**	0.958	0.97	0.93	0.97	0.94	0.95	0.03	0.06	0.03	0.04	0.01	0.14	0.13	0.14	0.13	0.13	2.6	6.7	2.8	3.9	1.2	1	1	1	1	1
DR-27bbSTER		0.736	0.74	0.74	0.75	0.74	0.74	0.01	0.00	0.03	0.01	0.01	0.10	0.10	0.11	0.10	0.10	1.6	0.7	3.8	1.1	1.8	1	1	1	1	1
DR-28bbSTER		0.323	0.32	0.32	0.32	0.32	0.32	0.02	0.01	0.01	0.01	0.01	0.04	0.04	0.04	0.04	0.04	5.2	2.4	1.9	3.9	3.3	1	1	1	1	1
DR-29bbSTER		0.497	0.50	0.50	0.49	0.50	0.50	0.01	0.01	0.01	0.01	0.00	0.07	0.07	0.07	0.07	0.07	2.5	1.3	2.7	2.0	0.8	1	1	1	1	1
DR-TA21	**m/z231**	4.167	4.51	4.06	4.40	4.38	4.34	0.70	0.21	0.47	0.43	0.35	0.63	0.57	0.62	0.61	0.61	15.4	5.1	10.8	9.9	8.0	0	1	1	1	1
DR-TA26		0.435	0.44	0.46	0.44	0.43	0.44	0.01	0.05	0.01	0.01	0.01	0.06	0.06	0.06	0.06	0.06	1.5	10.5	1.2	1.2	3.1	1	1	1	1	1
DR-TA27		1.028	1.03	1.04	1.02	1.03	1.03	0.00	0.02	0.01	0.00	0.00	0.14	0.15	0.14	0.14	0.14	0.3	1.8	0.9	0.3	0.2	1	1	1	1	1
DR-2MP/1MP	**PAH**	2.144	2.14	2.16	2.15	2.15	2.15	0.00	0.03	0.00	0.01	0.01	0.30	0.30	0.30	0.30	0.30	0.0	1.3	0.2	0.4	0.5	1	1	1	1	1
DR-4MD/1MD		2.444	2.44	2.45	2.43	2.44	2.44	0.01	0.02	0.03	0.00	0.01	0.34	0.34	0.34	0.34	0.34	0.4	0.7	1.3	0.0	0.2	1	1	1	1	1
DR-C2dbt/C2phe		0.628	0.63	0.65	0.62	0.63	0.63	0.00	0.04	0.02	0.00	0.01	0.09	0.09	0.09	0.09	0.09	0.3	5.8	3.0	0.5	0.8	1	1	1	1	1
DR-C3dbt/C3phe		0.779	0.79	0.81	0.77	0.78	0.79	0.02	0.06	0.01	0.01	0.02	0.11	0.11	0.11	0.11	0.11	2.1	6.9	1.7	0.8	2.1	1	1	1	1	1
DR-C3dbt/C3chr		2.703	2.83	3.03	2.66	2.77	2.82	0.24	0.66	0.09	0.14	0.24	0.40	0.42	0.37	0.39	0.40	8.6	21.8	3.3	4.9	8.5	1	0	1	1	1
DR-Retene/C4phe		0.051	0.05	0.05	0.05	0.05	0.05	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	13.9	14.8	17.3	12.9	14.7	1	0	0	1	0
DR-BaF/4Mpy		0.458	0.46	0.46	0.46	0.46	0.46	0.01	0.00	0.00	0.00	0.00	0.06	0.06	0.06	0.06	0.06	1.1	0.7	0.6	0.2	0.1	1	1	1	1	1
DR-BbcF/4Mpy		0.275	0.28	0.28	0.28	0.28	0.28	0.01	0.01	0.00	0.01	0.01	0.04	0.04	0.04	0.04	0.04	2.3	2.5	1.6	2.7	2.3	1	1	1	1	1
DR-2Mpy/4Mpy		0.962	0.96	0.96	0.96	0.97	0.96	0.01	0.00	0.01	0.02	0.00	0.13	0.13	0.13	0.14	0.13	0.8	0.3	0.8	1.6	0.1	1	1	1	1	1
DR-1Mpy/4Mpy		0.925	0.93	0.92	0.95	0.93	0.93	0.01	0.00	0.05	0.00	0.01	0.13	0.13	0.13	0.13	0.13	0.8	0.4	5.3	0.1	1.5	1	1	1	1	1
DR-SES1/SES2	**m/z123**	1.623	1.62	1.65	1.67	1.67	1.65	0.00	0.05	0.10	0.09	0.06	0.23	0.23	0.23	0.23	0.23	0.2	3.3	6.0	5.6	3.7	1	1	1	1	1
DR-SES3/SES5		0.404	0.43	0.40	0.40	0.41	0.41	0.05	0.02	0.00	0.01	0.01	0.06	0.06	0.06	0.06	0.06	12.5	3.9	0.3	2.7	2.9	1	1	1	1	1
DR-SES4/SES6		0.891	0.97	0.94	0.90	0.93	0.94	0.16	0.11	0.02	0.07	0.09	0.14	0.13	0.13	0.13	0.13	16.3	11.5	2.7	7.5	9.6	0	1	1	1	1
DR-SES5/SES10		0.817	0.86	0.90	0.87	0.88	0.88	0.08	0.17	0.12	0.12	0.12	0.12	0.13	0.12	0.12	0.12	9.2	18.5	13.2	13.9	13.7	1	0	1	1	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2007-0017	06-Feb-2007	Emulsion from "TV-bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2. 2007-0023	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 3
3. 2007-0024	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 4
4. 2007-0033	07-Feb-2007	Oil sample collected at KV " Eigun"

Figure E.18: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0064) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: oljeprøve HeTest Date: 14–Mar–2007 Description: Bird feathers from wounded seagull (skårunge), Træna

Ratio Name		Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
			R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR–C28	**m/z191**	0.162	0.19	0.19	0.20	0.20	0.19	0.06	0.05	0.08	0.07	0.06	0.03	0.03	0.03	0.03	0.03	30.4	24.9	38.2	36.2	32.6	0	0	0	0	0
DR–C29		0.140	0.15	0.15	0.16	0.15	0.15	0.02	0.02	0.03	0.02	0.03	0.02	0.02	0.02	0.02	0.02	16.2	15.6	22.0	14.3	17.1	0	0	0	0	0
DR–C28C29		0.302	0.34	0.34	0.36	0.35	0.35	0.08	0.07	0.11	0.09	0.09	0.05	0.05	0.05	0.05	0.05	24.1	20.7	31.1	26.7	25.7	0	0	0	0	0
DR–27Ts		0.554	0.53	0.53	0.55	0.53	0.54	0.04	0.04	0.01	0.05	0.03	0.07	0.07	0.08	0.07	0.08	7.3	7.8	2.1	9.0	6.5	1	1	1	1	1
DR–28ab		0.096	0.12	0.11	0.12	0.12	0.12	0.05	0.02	0.04	0.04	0.04	0.02	0.02	0.02	0.02	0.02	41.8	20.9	35.6	34.8	33.6	0	0	0	0	0
DR–25nor30ab		0.053	0.06	0.05	0.06	0.06	0.06	0.02	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	25.8	5.0	8.8	18.8	14.9	0	1	1	0	0
DR–29Ts		0.156	0.16	0.16	0.16	0.16	0.16	0.01	0.00	0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.02	5.0	0.7	1.1	1.0	1.4	1	1	1	1	1
DR–30O		0.085	0.09	0.10	0.09	0.09	0.09	0.01	0.03	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	8.7	30.7	3.4	13.0	14.5	1	0	1	1	0
DR–30G		0.113	0.13	0.12	0.12	0.12	0.12	0.03	0.01	0.02	0.01	0.02	0.02	0.02	0.02	0.02	0.02	20.6	4.7	16.3	11.7	13.5	0	1	0	1	1
DR–29ab		0.915	0.91	0.93	0.89	0.92	0.91	0.01	0.03	0.05	0.01	0.00	0.13	0.13	0.12	0.13	0.13	1.5	3.0	5.2	1.3	0.5	1	1	1	1	1
DR–30d		0.039	0.05	0.04	0.04	0.04	0.04	0.02	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	32.9	7.2	9.2	12.3	16.0	0	1	1	1	0
DR–29aaS	**m/z217**	0.939	0.91	0.91	0.90	0.93	0.91	0.07	0.05	0.08	0.02	0.05	0.13	0.13	0.13	0.13	0.13	7.6	5.4	8.3	2.5	5.9	1	1	1	1	1
DR–29bb	**&218**	1.072	1.03	0.98	1.03	1.00	1.01	0.09	0.18	0.09	0.15	0.13	0.14	0.14	0.14	0.14	0.14	8.6	17.9	8.4	15.1	12.4	1	0	1	0	1
DR–27bbSTER		0.688	0.72	0.71	0.73	0.72	0.72	0.06	0.05	0.08	0.06	0.06	0.10	0.10	0.10	0.10	0.10	8.4	7.4	10.5	7.8	8.6	1	1	1	1	1
DR–28bbSTER		0.307	0.31	0.31	0.31	0.31	0.31	0.00	0.01	0.01	0.00	0.01	0.04	0.04	0.04	0.04	0.04	0.1	2.7	3.3	1.2	1.8	1	1	1	1	1
DR–29bbSTER		0.557	0.53	0.53	0.52	0.53	0.53	0.05	0.05	0.07	0.05	0.06	0.07	0.07	0.07	0.07	0.07	8.9	10.2	14.1	9.4	10.6	1	1	0	1	1
DR–TA21	**m/z231**	3.446	4.15	3.70	4.04	4.02	3.98	1.42	0.51	1.20	1.15	1.07	0.58	0.52	0.57	0.56	0.56	34.1	13.9	29.6	28.7	26.9	0	1	0	0	0
DR–TA26		0.428	0.43	0.46	0.43	0.43	0.44	0.01	0.05	0.01	0.00	0.02	0.06	0.06	0.06	0.06	0.06	3.0	12.0	2.7	0.3	4.6	1	1	1	1	1
DR–TA27		1.094	1.06	1.07	1.06	1.06	1.06	0.06	0.05	0.07	0.07	0.06	0.15	0.15	0.15	0.15	0.15	5.9	4.4	7.1	6.4	6.0	1	1	1	1	1
DR–2MP/1MP	**PAH**	2.137	2.14	2.15	2.14	2.14	2.15	0.01	0.04	0.01	0.02	0.02	0.30	0.30	0.30	0.30	0.30	0.3	1.7	0.6	0.8	0.8	1	1	1	1	1
DR–4MD/1MD		2.445	2.44	2.45	2.43	2.44	2.44	0.01	0.02	0.03	0.00	0.01	0.34	0.34	0.34	0.34	0.34	0.4	0.6	1.3	0.0	0.3	1	1	1	1	1
DR–C2dbt/C2phe		0.635	0.63	0.65	0.62	0.63	0.63	0.01	0.03	0.03	0.00	0.00	0.09	0.09	0.09	0.09	0.09	1.5	4.6	4.2	0.7	0.4	1	1	1	1	1
DR–C3dbt/C3phe		0.788	0.79	0.81	0.78	0.79	0.79	0.01	0.05	0.02	0.00	0.01	0.11	0.11	0.11	0.11	0.11	1.0	5.8	2.8	0.3	1.0	1	1	1	1	1
DR–C3dbt/C3chr		2.387	2.67	2.88	2.50	2.61	2.66	0.56	0.98	0.23	0.45	0.56	0.37	0.40	0.35	0.37	0.37	21.0	34.0	9.2	17.4	20.8	0	0	1	0	0
DR–Retene/C4phe		0.035	0.04	0.04	0.04	0.04	0.04	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	25.2	24.3	21.8	26.2	24.4	0	0	0	0	0
DR–BaF/4Mpy		0.484	0.47	0.47	0.47	0.47	0.47	0.02	0.03	0.03	0.03	0.03	0.07	0.07	0.07	0.07	0.07	4.5	6.3	6.2	5.7	5.7	1	1	1	1	1
DR–BbcF/4Mpy		0.286	0.28	0.28	0.28	0.28	0.28	0.00	0.00	0.01	0.00	0.00	0.04	0.04	0.04	0.04	0.04	1.6	1.4	2.3	1.2	1.6	1	1	1	1	1
DR–2Mpy/4Mpy		0.946	0.95	0.95	0.95	0.96	0.95	0.01	0.01	0.01	0.03	0.01	0.13	0.13	0.13	0.13	0.13	0.8	1.4	0.8	3.2	1.6	1	1	1	1	1
DR–1Mpy/4Mpy		0.911	0.92	0.92	0.94	0.92	0.92	0.02	0.01	0.06	0.01	0.03	0.13	0.13	0.13	0.13	0.13	2.3	1.1	6.8	1.6	3.0	1	1	1	1	1
DR–SES1/SES2	**m/z123**	1.630	1.62	1.65	1.68	1.67	1.66	0.01	0.05	0.09	0.09	0.05	0.23	0.23	0.23	0.23	0.23	0.7	2.9	5.5	5.1	3.2	1	1	1	1	1
DR–SES3/SES5		0.383	0.42	0.39	0.39	0.40	0.40	0.08	0.01	0.02	0.03	0.03	0.06	0.05	0.05	0.06	0.06	17.9	1.5	5.2	8.1	8.4	0	1	1	1	1
DR–SES4/SES6		0.950	1.00	0.97	0.93	0.95	0.97	0.10	0.05	0.03	0.01	0.03	0.14	0.14	0.13	0.13	0.14	9.8	5.0	3.7	1.0	3.2	1	1	1	1	1
DR–SES5/SES10		0.800	0.85	0.89	0.87	0.87	0.87	0.10	0.18	0.13	0.14	0.14	0.12	0.12	0.12	0.12	0.12	11.2	20.5	15.3	15.9	15.8	1	0	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2007–0017	06–Feb–2007	Emulsion from "TV–bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2. 2007–0023	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 3
3. 2007–0024	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 4
4. 2007–0033	07–Feb–2007	Oil sample collected at KV " Eigun"

Figure E.19: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0xxx) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007-0065 Test Date: 08-Feb-2007 Description: Oil klatt, Ivasanden, Ulstein

Ratio Name		Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
			R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR-C28	**m/z191**	0.188	0.20	0.20	0.21	0.21	0.21	0.03	0.02	0.05	0.05	0.04	0.03	0.03	0.03	0.03	0.03	15.8	10.2	23.8	21.7	18.0	0	1	0	0	0
DR-C29		0.152	0.16	0.16	0.16	0.16	0.16	0.01	0.01	0.02	0.01	0.01	0.02	0.02	0.02	0.02	0.02	8.2	7.5	14.0	6.3	9.0	1	1	0	1	1
DR-C28C29		0.340	0.36	0.36	0.38	0.37	0.37	0.05	0.03	0.07	0.06	0.05	0.05	0.05	0.05	0.05	0.05	12.5	9.0	19.5	15.1	14.1	1	1	0	0	0
DR-27Ts		0.575	0.55	0.54	0.56	0.54	0.55	0.06	0.06	0.03	0.07	0.06	0.08	0.08	0.08	0.08	0.08	10.9	11.4	5.7	12.6	10.1	1	1	1	1	1
DR-28ab		0.097	0.12	0.11	0.12	0.12	0.12	0.05	0.02	0.04	0.04	0.04	0.02	0.02	0.02	0.02	0.02	41.2	20.2	35.0	34.2	33.0	0	0	0	0	0
DR-25nor30ab		0.032	0.05	0.04	0.04	0.05	0.05	0.04	0.02	0.03	0.03	0.03	0.01	0.01	0.01	0.01	0.01	72.7	53.9	57.4	66.5	63.0	0	0	0	0	0
DR-29Ts		0.170	0.17	0.16	0.16	0.16	0.16	0.01	0.01	0.02	0.01	0.01	0.02	0.02	0.02	0.02	0.02	3.4	7.7	9.5	7.4	7.0	1	1	1	1	1
DR-30O		0.092	0.09	0.10	0.09	0.09	0.10	0.00	0.02	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.0	22.1	5.4	4.2	5.8	1	0	1	1	1
DR-30G		0.114	0.13	0.12	0.12	0.12	0.12	0.03	0.00	0.02	0.01	0.02	0.02	0.02	0.02	0.02	0.02	19.9	3.9	15.6	10.9	12.8	0	1	0	1	1
DR-29ab		1.019	0.96	0.98	0.94	0.97	0.96	0.12	0.08	0.15	0.09	0.11	0.13	0.14	0.13	0.14	0.14	12.2	7.7	16.0	9.4	11.3	1	1	0	1	1
DR-30d		0.041	0.05	0.04	0.04	0.04	0.04	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	26.9	1.0	3.0	6.1	9.8	0	1	1	1	1
DR-29aaS	**m/z217**	0.956	0.91	0.92	0.91	0.94	0.92	0.09	0.07	0.09	0.04	0.07	0.13	0.13	0.13	0.13	0.13	9.3	7.2	10.1	4.3	7.7	1	1	1	1	1
DR-29bb	**&218**	1.007	0.99	0.95	1.00	0.96	0.98	0.02	0.11	0.02	0.09	0.06	0.14	0.13	0.14	0.13	0.14	2.4	11.7	2.2	8.9	6.2	1	1	1	1	1
DR-27bbSTER		0.680	0.71	0.71	0.72	0.71	0.71	0.07	0.06	0.08	0.06	0.07	0.10	0.10	0.10	0.10	0.10	9.6	8.6	11.7	9.0	9.8	1	1	1	1	1
DR-28bbSTER		0.315	0.31	0.32	0.32	0.31	0.31	0.01	0.00	0.00	0.00	0.00	0.04	0.04	0.04	0.04	0.04	2.7	0.1	0.6	1.4	0.9	1	1	1	1	1
DR-29bbSTER		0.552	0.53	0.53	0.52	0.53	0.53	0.04	0.05	0.07	0.05	0.05	0.07	0.07	0.07	0.07	0.07	8.1	9.3	13.2	8.6	9.8	1	1	1	1	1
DR-TA21	**m/z231**	4.131	4.50	4.05	4.39	4.37	4.32	0.73	0.17	0.51	0.47	0.38	0.63	0.57	0.61	0.61	0.61	16.3	4.3	11.6	10.7	8.9	0	1	1	1	1
DR-TA26		0.355	0.40	0.42	0.40	0.39	0.40	0.09	0.13	0.08	0.07	0.09	0.06	0.06	0.06	0.05	0.06	21.6	30.4	21.2	18.9	23.2	0	0	0	0	0
DR-TA27		1.118	1.07	1.08	1.07	1.07	1.07	0.09	0.07	0.10	0.09	0.09	0.15	0.15	0.15	0.15	0.15	8.1	6.6	9.3	8.6	8.1	1	1	1	1	1
DR-2MP/1MP	**PAH**	2.144	2.14	2.16	2.15	2.15	2.15	0.00	0.03	0.00	0.01	0.01	0.30	0.30	0.30	0.30	0.30	0.0	1.3	0.2	0.4	0.5	1	1	1	1	1
DR-4MD/1MD		2.482	2.46	2.47	2.45	2.46	2.46	0.05	0.02	0.07	0.04	0.04	0.34	0.35	0.34	0.34	0.34	1.9	0.8	2.8	1.5	1.8	1	1	1	1	1
DR-C2dbt/C2phe		0.655	0.64	0.66	0.63	0.64	0.64	0.03	0.01	0.04	0.02	0.02	0.09	0.09	0.09	0.09	0.09	4.5	1.6	7.1	3.7	3.4	1	1	1	1	1
DR-C3dbt/C3phe		0.822	0.81	0.83	0.79	0.80	0.81	0.03	0.01	0.06	0.04	0.03	0.11	0.12	0.11	0.11	0.11	3.2	1.5	7.0	4.6	3.3	1	1	1	1	1
DR-C3dbt/C3chr		3.125	3.04	3.24	2.87	2.98	3.03	0.18	0.24	0.51	0.28	0.18	0.43	0.45	0.40	0.42	0.42	5.9	7.4	17.7	9.5	6.0	1	1	0	1	1
DR-Retene/C4phe		0.048	0.05	0.05	0.05	0.05	0.05	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	6.7	7.6	10.1	5.7	7.5	1	1	1	1	1
DR-BaF/4Mpy		0.452	0.46	0.45	0.45	0.45	0.45	0.01	0.00	0.00	0.01	0.01	0.06	0.06	0.06	0.06	0.06	2.4	0.6	0.7	1.1	1.2	1	1	1	1	1
DR-BbcF/4Mpy		0.265	0.27	0.27	0.27	0.27	0.27	0.02	0.02	0.01	0.02	0.02	0.04	0.04	0.04	0.04	0.04	6.1	6.3	5.4	6.5	6.1	1	1	1	1	1
DR-2Mpy/4Mpy		0.950	0.95	0.95	0.95	0.96	0.96	0.00	0.01	0.00	0.03	0.01	0.13	0.13	0.13	0.13	0.13	0.5	1.0	0.5	2.9	1.2	1	1	1	1	1
DR-1Mpy/4Mpy		0.905	0.92	0.91	0.94	0.92	0.92	0.03	0.02	0.07	0.02	0.03	0.13	0.13	0.13	0.13	0.13	2.9	1.7	7.4	2.3	3.6	1	1	1	1	1
DR-SES1/SES2	**m/z123**	1.547	1.58	1.61	1.63	1.63	1.62	0.07	0.13	0.18	0.17	0.14	0.22	0.23	0.23	0.23	0.23	4.6	8.1	10.8	10.3	8.5	1	1	1	1	1
DR-SES3/SES5		0.372	0.41	0.38	0.39	0.39	0.39	0.09	0.02	0.03	0.04	0.04	0.06	0.05	0.05	0.06	0.06	20.7	4.4	8.0	10.9	11.2	0	1	1	1	1
DR-SES4/SES6		0.924	0.99	0.96	0.92	0.94	0.95	0.12	0.07	0.01	0.04	0.06	0.14	0.13	0.13	0.13	0.13	12.6	7.8	1.0	3.8	5.9	1	1	1	1	1
DR-SES5/SES10		0.596	0.75	0.79	0.76	0.77	0.77	0.30	0.39	0.34	0.34	0.34	0.10	0.11	0.11	0.11	0.11	40.1	49.0	44.0	44.6	44.5	0	0	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2007-0017	06-Feb-2007	Emulsion from "TV-bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2. 2007-0023	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 3
3. 2007-0024	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 4
4. 2007-0033	07-Feb-2007	Oil sample collected at KV " Eigun"

Figure E.20: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0065) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007–0023 Test Date: 07–Feb–2007 Description: Oil from shipwreck – "Server": Sample from Tank 3

Ratio Name		Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
			R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR–C28	m/z191	0.209	0.21	0.21	0.22	0.22	0.22	0.01	0.00	0.03	0.03	0.02	0.03	0.03	0.03	0.03	0.03	5.6	0.0	13.7	11.5	7.9	1	1	1	1	1
DR–C29		0.163	0.16	0.16	0.17	0.16	0.16	0.00	0.00	0.01	0.00	0.00	0.02	0.02	0.02	0.02	0.02	0.6	0.0	6.5	1.2	1.5	1	1	1	1	1
DR–C28C29		0.372	0.38	0.37	0.39	0.38	0.38	0.01	0.00	0.04	0.02	0.02	0.05	0.05	0.05	0.05	0.05	3.5	0.0	10.6	6.1	5.1	1	1	1	1	1
DR–27Ts		0.513	0.51	0.51	0.53	0.51	0.52	0.00	0.00	0.03	0.01	0.01	0.07	0.07	0.07	0.07	0.07	0.6	0.0	5.8	1.2	1.3	1	1	1	1	1
DR–28ab		0.119	0.13	0.12	0.13	0.13	0.13	0.03	0.00	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	21.4	0.0	15.0	14.2	13.0	0	1	0	0	1
DR–25nor30ab		0.055	0.06	0.06	0.06	0.06	0.06	0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	20.8	0.0	3.8	13.8	9.9	0	1	1	1	1
DR–29Ts		0.158	0.16	0.16	0.16	0.16	0.16	0.01	0.00	0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.02	4.2	0.0	1.8	0.2	0.7	1	1	1	1	1
DR–30O		0.115	0.10	0.12	0.10	0.11	0.11	0.02	0.00	0.03	0.02	0.02	0.01	0.02	0.01	0.01	0.01	22.1	0.0	27.4	17.9	16.4	0	1	0	0	0
DR–30G		0.119	0.13	0.12	0.13	0.12	0.12	0.02	0.00	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.02	16.0	0.0	11.7	7.0	8.9	0	1	1	1	1
DR–29ab		0.943	0.92	0.94	0.91	0.94	0.93	0.04	0.00	0.07	0.02	0.03	0.13	0.13	0.13	0.13	0.13	4.5	0.0	8.3	1.7	3.6	1	1	1	1	1
DR–30d		0.042	0.05	0.04	0.04	0.04	0.04	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	25.9	0.0	2.0	5.1	8.8	0	1	1	1	1
DR–29aaS	m/z217	0.890	0.88	0.89	0.88	0.90	0.89	0.02	0.00	0.03	0.03	0.00	0.12	0.12	0.12	0.13	0.12	2.1	0.0	2.9	2.9	0.5	1	1	1	1	1
DR–29bb	&218	0.896	0.94	0.90	0.94	0.91	0.92	0.09	0.00	0.09	0.02	0.05	0.13	0.13	0.13	0.13	0.13	9.3	0.0	9.4	2.8	5.5	1	1	1	1	1
DR–27bbSTER		0.741	0.74	0.74	0.75	0.74	0.75	0.01	0.00	0.02	0.00	0.01	0.10	0.10	0.11	0.10	0.10	1.0	0.0	3.1	0.4	1.1	1	1	1	1	1
DR–28bbSTER		0.316	0.31	0.32	0.32	0.31	0.31	0.01	0.00	0.00	0.00	0.00	0.04	0.04	0.04	0.04	0.04	2.8	0.0	0.5	1.5	0.9	1	1	1	1	1
DR–29bbSTER		0.503	0.51	0.50	0.49	0.50	0.50	0.01	0.00	0.02	0.00	0.00	0.07	0.07	0.07	0.07	0.07	1.2	0.0	3.9	0.8	0.5	1	1	1	1	1
DR–TA21	m/z231	3.959	4.41	3.96	4.30	4.28	4.24	0.90	0.00	0.68	0.64	0.56	0.62	0.55	0.60	0.60	0.59	20.5	0.0	15.9	15.0	13.1	0	1	0	0	1
DR–TA26		0.483	0.46	0.48	0.46	0.46	0.47	0.04	0.00	0.04	0.05	0.03	0.06	0.07	0.06	0.06	0.07	9.0	0.0	9.3	11.7	7.4	1	1	1	1	1
DR–TA27		1.046	1.04	1.05	1.03	1.04	1.04	0.02	0.00	0.03	0.02	0.02	0.15	0.15	0.14	0.15	0.15	1.5	0.0	2.7	2.0	1.6	1	1	1	1	1
DR–2MP/1MP	PAH	2.172	2.16	2.17	2.16	2.16	2.16	0.03	0.00	0.02	0.02	0.02	0.30	0.30	0.30	0.30	0.30	1.3	0.0	1.1	0.9	0.8	1	1	1	1	1
DR–4MD/1MD		2.461	2.45	2.46	2.44	2.45	2.45	0.03	0.00	0.05	0.02	0.02	0.34	0.34	0.34	0.34	0.34	1.1	0.0	1.9	0.7	0.9	1	1	1	1	1
DR–C2dbt/C2phe		0.665	0.65	0.67	0.64	0.65	0.65	0.04	0.00	0.06	0.03	0.03	0.09	0.09	0.09	0.09	0.09	6.1	0.0	8.7	5.3	5.0	1	1	1	1	1
DR–C3dbt/C3phe		0.834	0.81	0.83	0.80	0.81	0.81	0.04	0.00	0.07	0.05	0.04	0.11	0.12	0.11	0.11	0.11	4.7	0.0	8.5	6.1	4.8	1	1	1	1	1
DR–C3dbt/C3chr		3.365	3.16	3.36	2.99	3.10	3.15	0.42	0.00	0.75	0.52	0.42	0.44	0.47	0.42	0.43	0.44	13.2	0.0	25.0	16.9	13.4	1	1	0	0	1
DR–Retene/C4phe		0.044	0.04	0.04	0.04	0.04	0.04	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.9	0.0	2.5	1.9	0.1	1	1	1	1	1
DR–BaF/4Mpy		0.455	0.46	0.45	0.45	0.46	0.46	0.01	0.00	0.00	0.00	0.00	0.06	0.06	0.06	0.06	0.06	1.8	0.0	0.1	0.5	0.6	1	1	1	1	1
DR–BbcF/4Mpy		0.282	0.28	0.28	0.28	0.28	0.28	0.00	0.00	0.00	0.00	0.00	0.04	0.04	0.04	0.04	0.04	0.2	0.0	0.9	0.2	0.2	1	1	1	1	1
DR–2Mpy/4Mpy		0.959	0.96	0.96	0.96	0.97	0.96	0.01	0.00	0.00	0.02	0.00	0.13	0.13	0.13	0.14	0.13	0.6	0.0	0.5	1.8	0.2	1	1	1	1	1
DR–1Mpy/4Mpy		0.921	0.93	0.92	0.95	0.92	0.93	0.01	0.00	0.05	0.00	0.02	0.13	0.13	0.13	0.13	0.13	1.2	0.0	5.7	0.5	1.9	1	1	1	1	1
DR–SES1/SES2	m/z123	1.677	1.65	1.68	1.70	1.70	1.68	0.06	0.00	0.05	0.04	0.01	0.23	0.23	0.24	0.24	0.24	3.5	0.0	2.7	2.2	0.4	1	1	1	1	1
DR–SES3/SES5		0.389	0.42	0.39	0.40	0.40	0.40	0.07	0.00	0.01	0.03	0.03	0.06	0.05	0.06	0.06	0.06	16.3	0.0	3.6	6.5	6.8	0	1	1	1	1
DR–SES4/SES6		0.999	1.02	1.00	0.96	0.98	0.99	0.05	0.00	0.08	0.04	0.02	0.14	0.14	0.13	0.14	0.14	4.8	0.0	8.7	4.0	1.9	1	1	1	1	1
DR–SES5/SES10		0.983	0.94	0.98	0.96	0.96	0.96	0.09	0.00	0.05	0.04	0.05	0.13	0.14	0.13	0.13	0.13	9.3	0.0	5.3	4.6	4.8	1	1	1	1	1

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2007–0017	06–Feb–2007	Emulsion from "TV–bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2. 2007–0023	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 3
3. 2007–0024	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 4
4. 2007–0033	07–Feb–2007	Oil sample collected at KV " Eigun"

Figure E.21: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0023) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting																											Calculated by: Uswatun H.I. Kamalia
Spill Sample SINTEF ID: 2007-0066 Test Date: 08-Feb-2007 Description: Bird feathers from gannets (nr. 3), Ivasanden, Ulstein																											
Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*					
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4RA		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	
DR-C28 **m/z191**	0.175	0.20	0.19	0.21	0.20	0.20	0.05	0.03	0.06	0.06	0.05	0.03	0.03	0.03	0.03	0.03	22.9	17.3	30.8	28.7	25.1	0	0	0	0	0	
DR-C29	0.135	0.15	0.15	0.15	0.15	0.15	0.03	0.03	0.04	0.03	0.03	0.02	0.02	0.02	0.02	0.02	19.6	19.0	25.4	17.8	20.5	0	0	0	0	0	
DR-C28C29	0.310	0.35	0.34	0.36	0.35	0.35	0.07	0.06	0.10	0.09	0.08	0.05	0.05	0.05	0.05	0.05	21.5	18.0	28.5	24.1	23.1	0	0	0	0	0	
DR-27Ts	0.571	0.54	0.54	0.56	0.54	0.55	0.06	0.06	0.03	0.06	0.05	0.08	0.08	0.08	0.08	0.08	10.3	10.8	5.1	12.0	9.5	1	1	1	1	1	
DR-28ab	0.114	0.13	0.12	0.13	0.13	0.12	0.03	0.00	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	25.6	4.3	19.2	18.5	17.2	0	1	0	0	0	
DR-25nor30ab	0.055	0.06	0.06	0.06	0.06	0.06	0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	22.4	1.5	5.3	15.3	11.5	0	1	1	0	1	
DR-29Ts	0.155	0.16	0.16	0.16	0.16	0.16	0.01	0.00	0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.02	5.7	1.5	0.4	1.7	2.1	1	1	1	1	1	
DR-30O	0.087	0.09	0.10	0.09	0.09	0.09	0.01	0.03	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	6.0	28.0	0.6	10.2	11.8	1	0	1	1	1	
DR-30G	0.115	0.13	0.12	0.12	0.12	0.12	0.02	0.00	0.02	0.01	0.01	0.02	0.02	0.02	0.02	0.02	19.2	3.3	15.0	10.3	12.1	0	1	0	1	1	
DR-29ab	0.948	0.92	0.95	0.91	0.94	0.93	0.05	0.00	0.08	0.02	0.04	0.13	0.13	0.13	0.13	0.13	5.0	0.5	8.7	2.2	4.0	1	1	1	1	1	
DR-30d	0.044	0.05	0.04	0.04	0.04	0.04	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	20.7	5.3	3.3	0.1	3.6	0	1	1	1	1	
DR-29aaS **m/z217**	0.835	0.85	0.86	0.85	0.88	0.86	0.04	0.05	0.03	0.08	0.05	0.12	0.12	0.12	0.12	0.12	4.2	6.3	3.4	9.2	5.8	1	1	1	1	1	
DR-29bb **&218**	0.954	0.97	0.93	0.97	0.94	0.95	0.03	0.06	0.03	0.03	0.01	0.14	0.13	0.14	0.13	0.13	3.0	6.3	3.1	3.6	0.9	1	1	1	1	1	
DR-27bbSTER	0.654	0.70	0.70	0.71	0.70	0.70	0.09	0.09	0.11	0.09	0.09	0.10	0.10	0.10	0.10	0.10	13.3	12.4	15.5	12.8	13.5	1	1	0	1	1	
DR-28bbSTER	0.325	0.32	0.32	0.32	0.32	0.32	0.02	0.01	0.01	0.01	0.01	0.04	0.04	0.04	0.04	0.04	5.8	3.0	2.4	4.5	3.9	1	1	1	1	1	
DR-29bbSTER	0.560	0.53	0.53	0.52	0.53	0.53	0.05	0.06	0.08	0.05	0.06	0.07	0.07	0.07	0.07	0.07	9.6	10.8	14.7	10.1	11.3	1	1	0	1	1	
DR-TA21 **m/z231**	3.700	4.28	3.83	4.17	4.15	4.11	1.16	0.26	0.94	0.90	0.82	0.60	0.54	0.58	0.58	0.58	27.1	6.8	22.6	21.7	19.8	0	1	0	0	0	
DR-TA26	0.400	0.42	0.44	0.42	0.42	0.42	0.04	0.08	0.04	0.03	0.05	0.06	0.06	0.06	0.06	0.06	9.7	18.7	9.4	7.0	11.3	1	0	1	1	1	
DR-TA27	1.114	1.07	1.08	1.07	1.07	1.07	0.08	0.07	0.10	0.09	0.08	0.15	0.15	0.15	0.15	0.15	7.8	6.3	9.0	8.3	7.8	1	1	1	1	1	
DR-2MP/1MP **PAH**	2.077	2.11	2.12	2.11	2.11	2.12	0.07	0.10	0.07	0.08	0.08	0.30	0.30	0.30	0.30	0.30	3.2	4.5	3.4	3.6	3.7	1	1	1	1	1	
DR-4MD/1MD	2.390	2.41	2.43	2.40	2.42	2.41	0.04	0.07	0.02	0.05	0.05	0.34	0.34	0.34	0.34	0.34	1.8	2.9	1.0	2.2	2.0	1	1	1	1	1	
DR-C2dbt/C2phe	0.637	0.63	0.65	0.62	0.63	0.63	0.01	0.03	0.03	0.01	0.00	0.09	0.09	0.09	0.09	0.09	1.7	4.4	4.3	0.9	0.6	1	1	1	1	1	
DR-C3dbt/C3phe	0.810	0.80	0.82	0.79	0.80	0.80	0.01	0.02	0.04	0.03	0.02	0.11	0.12	0.11	0.11	0.11	1.8	2.9	5.6	3.2	1.9	1	1	1	1	1	
DR-C3dbt/C3chr	3.723	3.34	3.54	3.17	3.28	3.33	0.78	0.36	1.11	0.88	0.78	0.47	0.50	0.44	0.46	0.47	23.3	10.1	34.9	26.9	23.4	0	1	0	0	0	
DR-Retene/C4phe	0.032	0.04	0.04	0.04	0.04	0.04	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	32.3	31.4	28.9	33.2	31.5	0	0	0	0	0	
DR-BaF/4Mpy	0.448	0.46	0.45	0.45	0.45	0.45	0.02	0.01	0.01	0.01	0.01	0.06	0.06	0.06	0.06	0.06	3.3	1.6	1.7	2.1	2.2	1	1	1	1	1	
DR-BbcF/4Mpy	0.258	0.27	0.27	0.27	0.27	0.27	0.02	0.02	0.02	0.02	0.02	0.04	0.04	0.04	0.04	0.04	8.7	8.9	8.0	9.1	8.7	1	1	1	1	1	
DR-2Mpy/4Mpy	0.960	0.96	0.96	0.96	0.97	0.96	0.01	0.00	0.01	0.02	0.00	0.13	0.13	0.13	0.14	0.13	0.6	0.0	0.5	1.8	0.2	1	1	1	1	1	
DR-1Mpy/4Mpy	0.909	0.92	0.92	0.94	0.92	0.92	0.02	0.01	0.07	0.02	0.03	0.13	0.13	0.13	0.13	0.13	2.5	1.3	7.0	1.8	3.2	1	1	1	1	1	
DR-SES1/SESn **m/z123**	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0	0	0	0	0	
DR-SES3/SES5	0.255	0.36	0.32	0.33	0.33	0.34	0.20	0.13	0.15	0.16	0.16	0.05	0.05	0.05	0.05	0.05	56.9	41.5	45.0	47.7	48.0	0	0	0	0	0	
DR-SES4/SES6	0.720	0.88	0.86	0.82	0.84	0.85	0.33	0.28	0.20	0.24	0.26	0.12	0.12	0.11	0.12	0.12	37.2	32.5	23.9	28.6	30.7	0	0	0	0	0	
DR-SES5/SES10	0.384	0.64	0.68	0.66	0.66	0.66	0.51	0.60	0.55	0.55	0.55	0.09	0.10	0.09	0.09	0.09	80.0	87.7	83.3	83.9	83.8	0	0	0	0	0	

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
1. 2007-0017	06-Feb-2007	Emulsion from "TV-bukta" by the lighthouse on Fedje. Sample from Sturla Dyregrov.
2. 2007-0023	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 3
3. 2007-0024	07-Feb-2007	Oil from shipwreck - "Server": Sample from Tank 4
4. 2007-0033	07-Feb-2007	Oil sample collected at KV " Eigun"

Figure E.22: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0066) and the reference samples.

Evaluation of The Diagnostic Ratio – MS Server Oil Spill Fingerprinting Calculated by: Uswatun H.I. Kamalia

Spill Sample SINTEF ID: 2007–0067 Test Date: 08–Feb–2007 Description: Bird feathers from guillemot / razorbills (nr. 4), Ivasanden, Ulstein

Ratio Name	Spill	Mean					Absolute Difference					Critical Difference					Percentage Difference					Flag*				
		R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA	R1	R2	R3	R4	RA
DR–C28 **m/z191**	0.177	0.20	0.19	0.21	0.21	0.20	0.04	0.03	0.06	0.06	0.05	0.03	0.03	0.03	0.03	0.03	22.2	16.7	30.1	28.1	24.4	0	0	0	0	0
DR–C29	0.142	0.15	0.15	0.16	0.15	0.15	0.02	0.02	0.03	0.02	0.02	0.02	0.02	0.02	0.02	0.02	14.3	13.7	20.2	12.5	15.2	0	1	0	1	0
DR–C28C29	0.319	0.35	0.35	0.37	0.36	0.36	0.07	0.05	0.09	0.08	0.07	0.05	0.05	0.05	0.05	0.05	18.8	15.4	25.8	21.4	20.4	0	0	0	0	0
DR–27Ts	0.563	0.54	0.54	0.55	0.53	0.54	0.05	0.05	0.02	0.06	0.04	0.08	0.08	0.08	0.07	0.08	8.8	9.4	3.6	10.6	8.1	1	1	1	1	1
DR–28ab	0.108	0.13	0.11	0.12	0.12	0.12	0.04	0.01	0.03	0.03	0.03	0.02	0.02	0.02	0.02	0.02	31.4	10.1	25.0	24.2	23.0	0	1	0	0	0
DR–25nor30ab	0.055	0.06	0.06	0.06	0.06	0.06	0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	22.1	1.3	5.0	15.0	11.2	0	1	1	0	1
DR–29Ts	0.172	0.17	0.16	0.16	0.16	0.17	0.01	0.01	0.02	0.01	0.01	0.02	0.02	0.02	0.02	0.02	4.4	8.6	10.4	8.4	7.9	1	1	1	1	1
DR–30O	0.088	0.09	0.10	0.09	0.09	0.09	0.00	0.03	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	5.0	27.1	0.3	9.3	10.9	1	0	1	1	1
DR–30G	0.116	0.13	0.12	0.12	0.12	0.12	0.02	0.00	0.02	0.01	0.01	0.02	0.02	0.02	0.02	0.02	18.1	2.2	13.9	9.2	11.0	0	1	1	1	1
DR–29ab	0.943	0.92	0.94	0.91	0.93	0.93	0.04	0.00	0.07	0.02	0.03	0.13	0.13	0.13	0.13	0.13	4.5	0.0	8.2	1.7	3.5	1	1	1	1	1
DR–30d	0.041	0.05	0.04	0.04	0.04	0.04	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	27.6	1.8	3.8	6.9	10.6	0	1	1	1	1
DR–29aaS **m/z217**	0.895	0.88	0.89	0.88	0.91	0.89	0.02	0.01	0.03	0.02	0.01	0.12	0.12	0.12	0.13	0.12	2.7	0.6	3.5	2.3	1.1	1	1	1	1	1
DR–29bb **&218**	1.023	1.00	0.96	1.00	0.97	0.98	0.04	0.13	0.04	0.10	0.08	0.14	0.13	0.14	0.14	0.14	4.0	13.2	3.8	10.5	7.8	1	1	1	1	1
DR–27bbSTER	0.642	0.69	0.69	0.70	0.69	0.70	0.11	0.10	0.12	0.10	0.11	0.10	0.10	0.10	0.10	0.10	15.3	14.3	17.5	14.8	15.5	0	0	0	0	0
DR–28bbSTER	0.323	0.31	0.32	0.32	0.32	0.32	0.02	0.01	0.01	0.01	0.01	0.04	0.04	0.04	0.04	0.04	5.0	2.2	1.7	3.7	3.2	1	1	1	1	1
DR–29bbSTER	0.575	0.54	0.54	0.53	0.54	0.54	0.07	0.07	0.09	0.07	0.07	0.08	0.08	0.07	0.08	0.08	12.2	13.4	17.3	12.7	13.9	1	1	0	1	1
DR–TA21 **m/z231**	3.713	4.29	3.84	4.18	4.16	4.11	1.15	0.25	0.93	0.89	0.80	0.60	0.54	0.58	0.58	0.58	26.8	6.4	22.2	21.3	19.5	0	1	0	0	0
DR–TA26	0.344	0.39	0.41	0.39	0.39	0.40	0.10	0.14	0.10	0.09	0.10	0.05	0.06	0.05	0.05	0.06	24.8	33.6	24.5	22.2	26.4	0	0	0	0	0
DR–TA27	1.106	1.07	1.08	1.06	1.07	1.07	0.07	0.06	0.09	0.08	0.08	0.15	0.15	0.15	0.15	0.15	7.0	5.5	8.2	7.5	7.1	1	1	1	1	1
DR–2MP/1MP **PAH**	2.107	2.13	2.14	2.13	2.13	2.13	0.04	0.07	0.04	0.05	0.05	0.30	0.30	0.30	0.30	0.30	1.7	3.0	2.0	2.2	2.2	1	1	1	1	1
DR–4MD/1MD	2.445	2.44	2.45	2.43	2.44	2.44	0.01	0.02	0.03	0.00	0.01	0.34	0.34	0.34	0.34	0.34	0.4	0.7	1.3	0.0	0.3	1	1	1	1	1
DR–C2dbt/C2phe	0.646	0.64	0.66	0.63	0.64	0.64	0.02	0.02	0.04	0.02	0.01	0.09	0.09	0.09	0.09	0.09	3.2	2.9	5.9	2.4	2.1	1	1	1	1	1
DR–C3dbt/C3phe	0.819	0.81	0.83	0.79	0.80	0.81	0.02	0.02	0.05	0.03	0.02	0.11	0.12	0.11	0.11	0.11	2.9	1.8	6.7	4.3	3.0	1	1	1	1	1
DR–C3dbt/C3chr	3.334	3.14	3.35	2.97	3.09	3.14	0.39	0.03	0.72	0.49	0.39	0.44	0.47	0.42	0.43	0.44	12.3	0.9	24.1	16.0	12.5	1	1	0	0	1
DR–Retene/C4phe	0.034	0.04	0.04	0.04	0.04	0.04	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	27.4	26.5	24.0	28.3	26.5	0	0	0	0	0
DR–BaF/4Mpy	0.449	0.46	0.45	0.45	0.45	0.45	0.01	0.01	0.01	0.01	0.01	0.06	0.06	0.06	0.06	0.06	3.1	1.3	1.4	1.8	1.9	1	1	1	1	1
DR–BbcF/4Mpy	0.275	0.28	0.28	0.28	0.28	0.28	0.01	0.01	0.00	0.01	0.01	0.04	0.04	0.04	0.04	0.04	2.4	2.6	1.7	2.8	2.4	1	1	1	1	1
DR–2Mpy/4Mpy	0.973	0.96	0.97	0.96	0.98	0.97	0.02	0.01	0.02	0.00	0.01	0.13	0.14	0.13	0.14	0.14	2.0	1.4	1.9	0.4	1.2	1	1	1	1	1
DR–1Mpy/4Mpy	0.907	0.92	0.91	0.94	0.92	0.92	0.03	0.01	0.07	0.02	0.03	0.13	0.13	0.13	0.13	0.13	2.7	1.5	7.2	2.0	3.4	1	1	1	1	1
DR–SES1/SES2 **m/z123**	1.532	1.58	1.60	1.63	1.62	1.61	0.09	0.15	0.19	0.18	0.15	0.22	0.22	0.23	0.23	0.23	5.5	9.0	11.7	11.3	9.4	1	1	1	1	1
DR–SES3/SES5	0.324	0.39	0.36	0.36	0.37	0.37	0.13	0.06	0.08	0.09	0.09	0.05	0.05	0.05	0.05	0.05	34.1	18.1	21.7	24.5	24.8	0	0	0	0	0
DR–SES4/SES6	0.813	0.93	0.91	0.86	0.89	0.90	0.23	0.19	0.10	0.15	0.17	0.13	0.13	0.12	0.12	0.13	25.2	20.5	11.8	16.5	18.6	0	0	1	0	0
DR–SES5/SES10	0.498	0.70	0.74	0.72	0.72	0.72	0.40	0.49	0.43	0.44	0.44	0.10	0.10	0.10	0.10	0.10	57.0	65.5	60.7	61.3	61.2	0	0	0	0	0

*0: %Diff > $r_{95\%}$; 1: %Diff <= $r_{95\%}$; $r_{95\%}$ = 14%

Reference Samples:

SINTEF ID	Test Date	Sample Description
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3. 2007–0024	07–Feb–2007	Oil from shipwreck – "Server": Sample from Tank 4
4. 2007–0033	07–Feb–2007	Oil sample collected at KV " Eigun"

Figure E.23: Evaluation of diagnostic ratio (CEN Methods) of "Server" case of the oil spill sample (SINTEF ID: 2007-0067) and the reference samples.

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