CHARACTERIZATION OF ORGANIC CONSTITUENTS OF ENVIRONMENTAL FILMS BY GC/MS

CHARACTERIZATION OF ORGANIC CONSTITUENTS OF ENVIRONMENTAL FILMS BY GC/MS

By

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A Thesis

Submitted to the School of Graduate Studies

in Partial Fulfilment of the Requirements

for the Degree

Master of Science

McMaster Univeristy

MASTER OF SCIENCE (2005) McMaster University

(Chemistry) Hamilton, Ontario

TITLE: Characterization of Organic Constituents of Environmental Films by GC/MS

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NUMBER OF PAGES: xviii, 144

ABSTRACT

The work of this thesis focuses on the further characterization of organic films that develop on the exterior and interior surfaces of windows in urban and rural areas. Previous work by our group has shown that these organic films contain organic contaminants (PAH, PCBs, OC pesticides, etc.), and air particulate material. Simulated precipitation experiments have shown that the organic film is easily washed off and that these contaminants enter surface waters, ultimately finding their way into sediments in rivers, lakes and oceans.

Samples of organic films on windows were collected at numerous sites in the Toronto area between July 2000 and July 2001. Previous work led to the quantification of over 85 target analytes within these film samples including, n-alkanes, n-alkanoic acids, n-alkanoic diacids, unsaturated alkanoic acids, aromatic carboxylic acids and resin acids.

Crude methanol extracts of these film samples were derivatized ($MeONH_2 \bullet HCl$ in pyridine, 37°C, 90 min. followed by N-trimethylsilyl-N-methyltrifluoroacetamide (MSTFA), 37°C, 30 min.) and analyzed by GC/MS in full scan EI^+ mode. Twenty seven compounds were positively identified with authentic standards, showing excellent matches to mass spectra and retention index values. These compounds included sugars (arabinose, glucose, fructose, sucrose, trehalose), sugar alcohols (xylitol, pinitol, quebrachitol, inositols), acids (glyceric, benzoic, fumaric, succinic, malic, adipic, azelaic) and a number of other unidentified derivatives. A total of 103 unique peaks were observed in 12 window film samples. It appears that these compounds are of plant origin

owing to the identification of plant sterols, β-sitosterol and stigmastanol. In addition, the wood combustion marker, levoglucosan, was identified in all but one film sample.

The patterns of polar compounds identified in these films are similar to recent findings of these substances in air particulate. The profiles of these polar compounds in three Hamilton PM_{10} samples were similar to literature reports.

The contribution of these newly identified compounds to the film exceeds or greatly exceeds the contribution of all previously identified chemical substances. There remains a significant amount of unidentified material in these films. The importance of these films lies in their pivotal role in the sequestering, transport and fate of organic contaminants in urban environments.

ACKNOWLEDGEMENTS

I would like to thank my supervisor Dr. B.E. McCarry for all of his guidance and support throughout this research project. I have learned so much from you over the course of my thesis not only about chemistry, but about myself as well. It has been a tremendous privilege for me to able work with you over the past few years.

I would also like to express my gratitude to the other members of our research group that I have worked side by side with. Thank you, Libia Saborido, Julia Jia, Sujan Fernando, Rong Yang, Brian Edwards, Tarlika Persaud and Jarrod Johnson for making my time in the lab a truly enjoyable experience.

I would also like to thank the people in the Mass Spectrometry Facility for all of their help and thanks to Dr. Don Hughes for running my NMR samples.

Last, but not least I would definitely like to thank everyone in the chemistry department here at McMaster that I have gotten to know over the years and wish you all the best in the future.

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LIST OF ABBREVIATIONS

DCM	Dichloromethane
GC/MS	Gas Chromatography/Mass Spectrometry
MSTFA	N-Trimethylsilyl-N-methyltrifluoroacetamide
MUM	Multimedia Urban Model
NMR	Nuclear Magnetic Resonance
OC	Organochlorine
PAH	Polycyclic Aromatic Hydrocarbon
PCA	Polychlorinated Alkanes
PCB	Polychlorinated Biphenyl
RI	Retention Index
RRF	Relative Response Factor
RSD	Relative Standard Deviation
SOC	Semi-volatile Organic Compound
STDEV	Standard Deviation
TIC	Total Ion Chromatogram
TMS	Trimethylsilyl
TOF	Time-of-Flight
VOC	Volatile Organic Compound

1.0 INTRODUCTION

1.1 Impervious Surfaces in the Environment

In the environment, surfaces can be classified as either being impervious or pervious/semi-pervious[47]. An impervious surface does not allow any water to permeate through and as a result the water along with any dissolved compounds ultimately ends up in the drainage systems[48]. Examples of impervious surfaces include roads, building walls, concrete, roofs and windows. A pervious/semi-pervious surface tends to allow water to permeate through them, such as the soils of lawns and gardens. Impervious surfaces can reach up to 98% coverage in some urban centres[47]; the percentage of land area covered by impervious surfaces is typically about 40% in North America.

1.2 Background Information

Studies of volatile organic compounds (VOC) and semi-volatile organic compounds (SOC) by Gustafson[48] and Halsall[49] reported elevated concentrations of these compounds at urban sites, while rural sites showed lower concentrations and smaller concentration changes with temperature.

Populations are becoming more and more urbanized worldwide; yet the role that the built environments have on the transport and fate of contaminants is not well understood. Relative to rural areas, urban areas show elevated concentrations of contaminants in virtually all media and a faster rate of transport of these contaminants to surface waters via storm water runoff[50]. The textbook pathways for contaminant transport of airborne contaminants in the environment are wet deposition and dry

deposition (air-water and air-soil transport)[60]. However, these pathways alone cannot fully explain the elevated concentrations of contaminants in urban areas[50]. Urban environments differ from rural environments by the presence of a greater number of impervious surfaces, much less vegetation and radically altered hydrologic regimes[59].

Diamond et al. hypothesized that organic films formed on urban impervious surfaces and acted as repositories for contaminants; in subsequent work they demonstrated the existence of an organic film on windows[40]. It was initially believed that the films developed on impervious surfaces via two routes:

(1) Direct deposition of primary gas-phase and particulate emissions

(2) Deposition of secondary reaction products of emissions

In route (1) organic compounds released directly from various emission sources would condense onto impervious surfaces. This phenomenon can be observed by the presence of an oily sheen on the surface of parking lots[51]. Other reports have shown that organic films are present on the surfaces of aerosols[52], fog droplets and snow flakes[54]. In route (2) primary emissions that have undergone chemical transformations in the gas-phase to give compounds with lower vapour pressures were proposed to condense onto impervious surfaces.

Once the film develops it is believed that fine particulate material can accumulate in the film due to the films "greasy" nature[55]. Gas-phase compounds can also partition into the organic film in a manner similar to that observed in open tube capillary GC columns[40]. Films in urban areas were found to be thicker (~20 nm) compared to those in

rural areas (5-10 fold less); thus urban films are probably capable of accumulating more gas and particle-phase chemicals[55,56].

1.3 Similarity of Organic Films to Air Particulate

Diamond et al. showed that the urban window films contained a wide range of organic contaminants, including polycyclic aromatic hydrocarbons (PAH), polychlorinated biphenyls (PCBs), organochlorine pesticides (OCs) and polychlorinated alkanes (PCAs). The relative abundances of PAH found in the organic window films was compared to that of different media found in the environment (June 1999)[40]. The levels of various PAH were determined in air (gas-phase), air (particle-phase), water, soil, vegetation and in the organic film. Figure 1-1 shows that the distribution pattern of PAH found in the film is quite similar to that of air particulate. The pattern of the PAH between retene (RE) and benzo[ghi]perylene (B[ghi]P) in Figure 1-1 is quite similar to the air particulate sample. The pattern of phenanthrene (PHE), anthracene (ANT), fluorene (FLU) and pyrene (PYR) in the film appears to be a mixture of both gas-phase and particle-phase aerosols. The film resembles "aged" urban since the more reactive PAH anthracene, benz[a]anthracene, benzo[a]pyrene and perylene have lower amounts that the unreactive PAH, chrysene, benzo[b]fluoranthene and perylene[40].

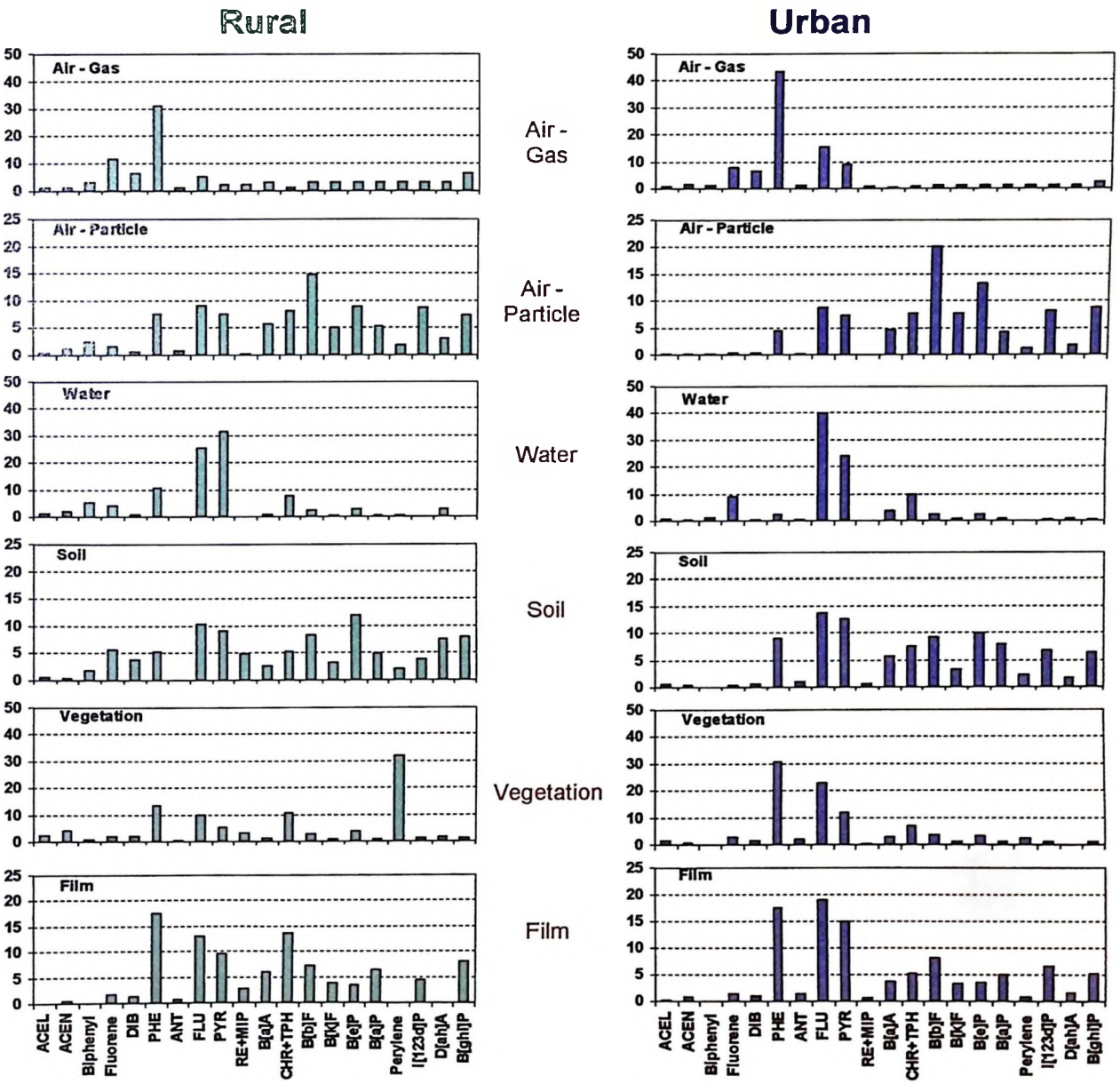


Figure 1-1. Comparison of PAH profiles found in window film and a variety of different media from urban and rural sites.

1.4 Indiscriminate Wash-off of Films and Potential Health Effects

The importance of these organic films in an environmental context results from their ability to act as sinks for a wide range of chemicals and particulate material in urban areas. Gingrich et al. found that about 70% of the organic film on a window was washed off under a simulated rainfall event[57,61]. Furthermore, the PAH, PCB and OC pesticide patterns found in the films before and after wash-off were essentially identical (see Figure 1-2 for PCB data). This observation was most unexpected; three-quarters of the film mass and three-quarters of the associated SOCs washed off together[58]. Clearly, the wash-off was non-selective and independent of the nature of the compounds contained within the organic film. The washed-off contaminants and any other chemicals in the film would end up in run-off, which finds its way into streams, rivers, lakes and oceans[59]. The film wash-off constitutes a new pathway for contaminants to enter the environment where they may exert adverse health effect on both humans and biota.

1.5 Multimedia Models

Multimedia models have been developed to describe the transformation, accumulation and movement of chemicals within and between compartments (media) in the environment. More complex model systems include, air, soil, water, biota and sediment as the key compartments[60].

Diamond et al. have developed a multimedia urban model (MUM)[61] to account for the role that organic films play in the transport of chemicals throughout the environment.

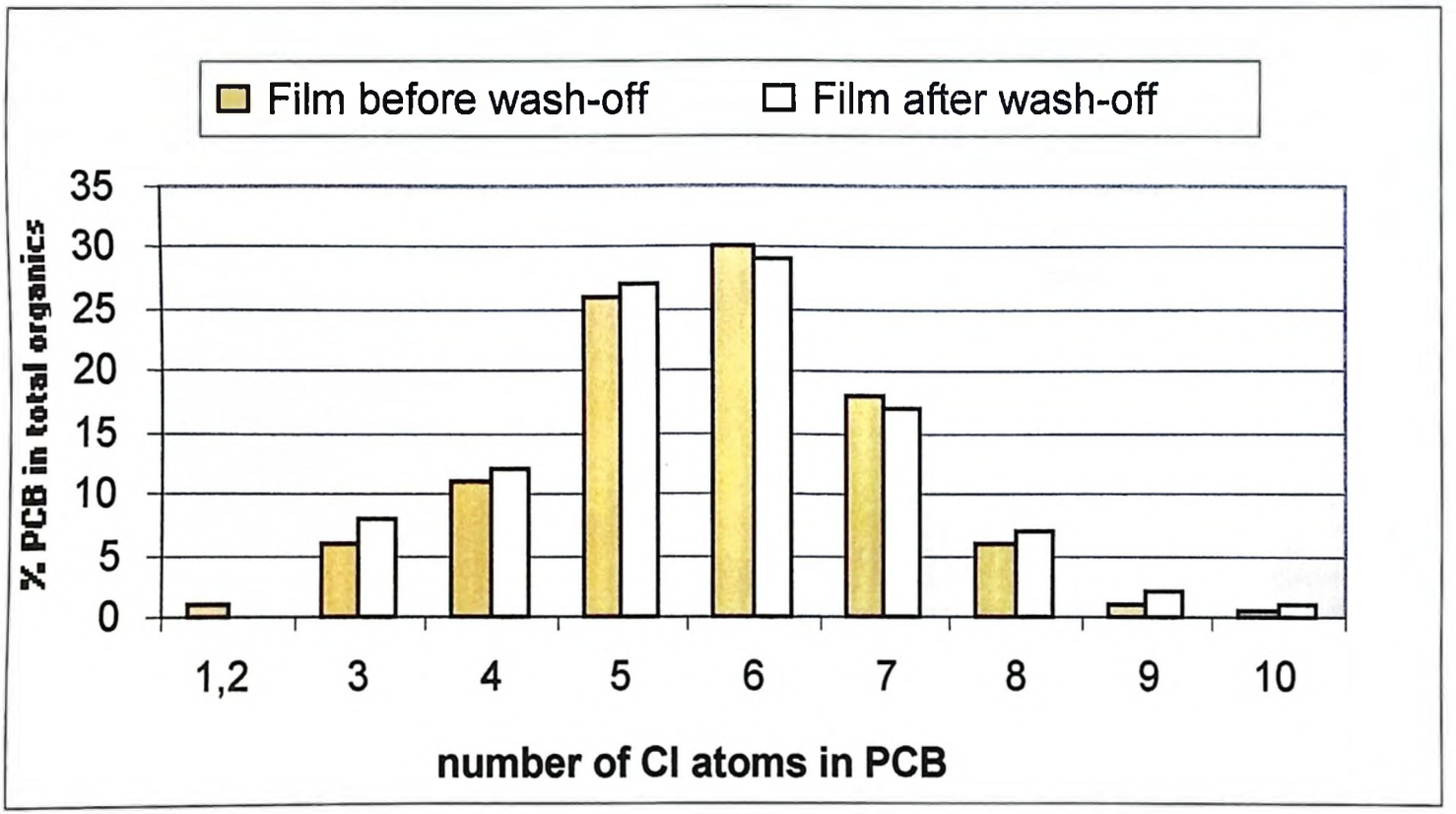


Figure 1-2. Distribution of PCBs in window films before and after wash-off by a simulated rainfall[57].

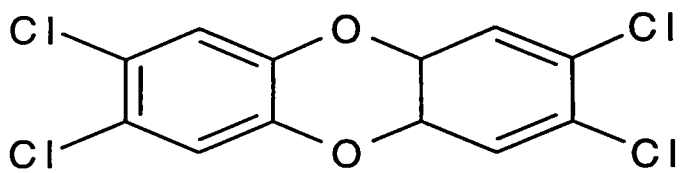
In their model six compartments were included: air, surface water, sediment, soil, vegetation and organic films on impervious surfaces. The MUM model, based on a Level III fugacity model developed by Mackay[62] assumes steady-state conditions. In summary, the most important observations based on the calculations performed by Diamond et al. were:

(1) Organic films had the highest concentrations of chemicals followed by sediments, soils and vegetation.

(2) The rates of chemical exchanges between the organic film and air were rapid, leading to increased chemical mobility.

(3) The film wash-off was the major route by which chemicals in the air would enter the surface waters.

2,3,7,8-Tetrachlorodibenzodioxin (TCDD) (Figure 1-3) was one of a number of key chemical contaminants that was used to evaluate the rates of movement using this multimedia transport model.



2,3,7,8-Tetrachloro-p-dibenzodioxin
(TCDD)

Figure 1-3. Structure of 2,3,7,8-Tetrachloro-p-dibenzodioxin.

Figure 1-4 shows that for every 1000 units of 2,3,7,8-tetrachlorodibenzodioxin that entered the air mass of the modelled system, 910 units would exit in the gas phase by advection. Of the remaining 90 units, 61 units would enter the water via the film of which 26 units would enter the sediment layer. By contrast wet and dry deposition, the classical routes for gas-phase and particle phase-contaminants to enter the water column only accounted for 5 units, i.e. 12 times less than the film wash-off. Those units of 2,3,7,8-tetrachlorodibenzodioxin that entered the soil remained there and did not move to the water column. Table 1-1 shows the different processes involved in the transport of chemicals to the different media.

Table 1-1. Processes Involved in the Transport of Contaminants in the Multimedia Model by Diamond et al[59].

Media	Process
Air-Film	gas diffusion wet deposition of gas wet deposition of particles dry deposition of particles
Film-Water	film washoff
Air-Vegetation	gas diffusion wet deposition of gas wet deposition of particles dry deposition of particles
Vegetation-Soil	canopy drip wax erosion litterfall
Soil-Vegetation	rainsplash

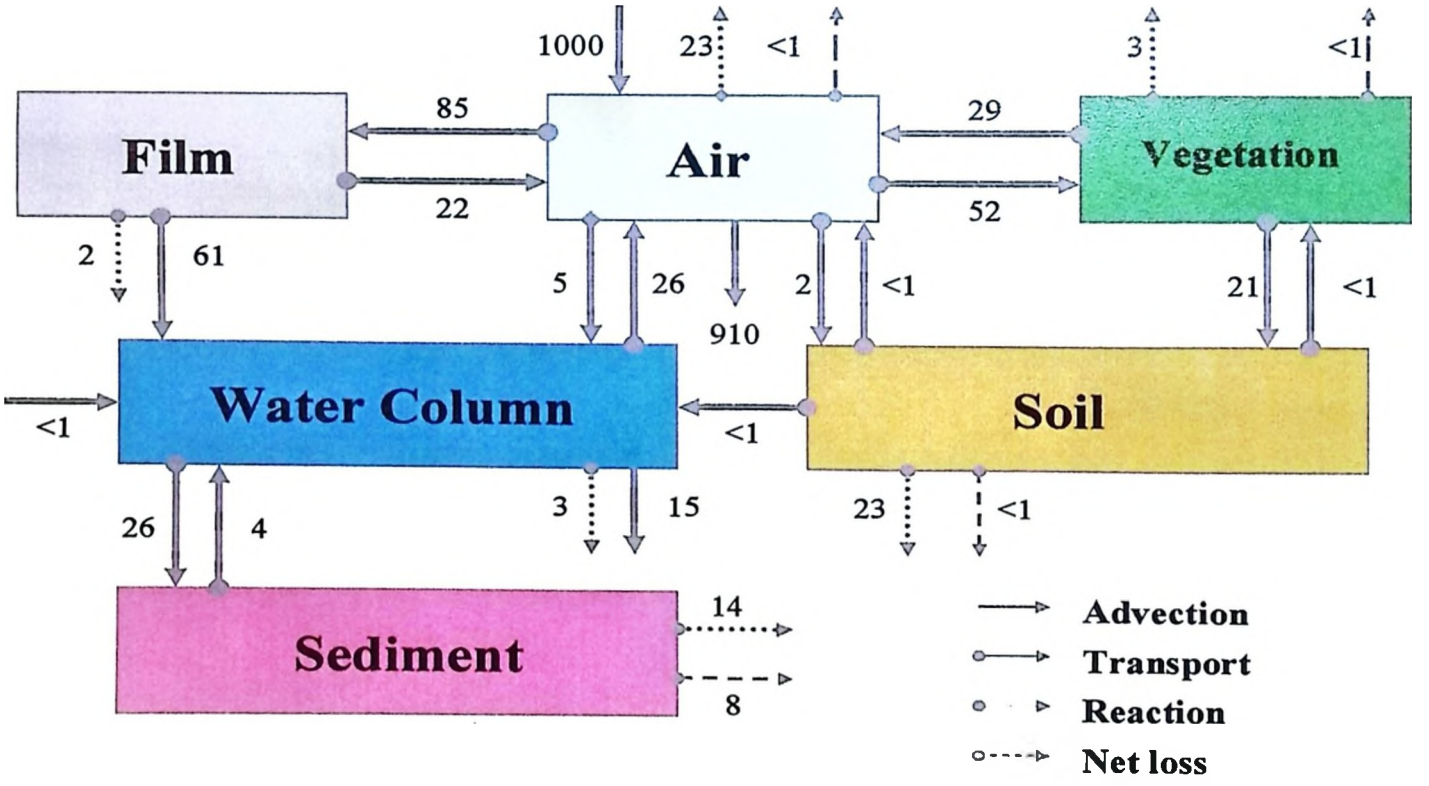


Figure 1-4. Multimedia model developed by Diamond et al.[61] showing the estimated rates of contaminant transport for 2,3,7,8-tetrachlorodibenozdioxin (mmol/h) in the environment.

It is clear that film acts the major pathway for contaminant transport between the air and the water in urban environments. These finding have major implications for both urban and rural environments. The non-selective wash-off of the contaminants from the films must be related to the chemical nature of the film. Therefore, determining the composition of the chemical constituents of the film should allow us to understand the unusual, indiscriminate wash-off process. The M.Sc. thesis work by Rachel Chen was the first attempt to solve this problem. The current thesis follows on the heels of Chen's thesis and attempts to address issues not answered by Chen.

1.6 Previous Work to Identify Bulk Components in the Film

1.6.1 Target Compound Analytes

Previous work in our lab to characterize the bulk chemical components of the film was performed by R. Chen and was based on a methodology developed by Cass and Simoneit[63-70]. Their approach involved the comprehensive analyses of non-polar and polar organic compounds found in 2.1 μm air particulate collected in Los Angeles in 1982[63-70]. In their procedure polar compounds were reacted with diazomethane (CH_2N_2) followed by GC/MS analysis[71-73]. Cass and Simoneit were primarily interested in source apportionment, which is based on the idea that each source of emissions may have a unique chemical signature and that ambient samples can be used to apportion the distribution and abundances of chemicals based on comparison to samples emitted by sources[74].

Figure 1-5 shows the chemical composition of the 2.1 μm air particulate sample. Organic compounds accounted for about 30% of the mass of the particulate material. The identified organic compounds only account for 10% of the total organic fraction; 90% of the organics remained unidentified. Most studies of aerosol samples are primarily concerned with identifying contaminants (e.g. PAH, PCBs and OC pesticides); however Figure 1-5 shows that these contaminants account for much less than 1% of the bulk extractable organic material.

Using the methodology developed by Cass and Simoneit, R. Chen was able to quantify over 85 target analytes in both indoor and outdoor window films[1]. The target analytes included n-alkanes (C_{11}-C_{36}), n-alkanoic acids (C_9-C_{31}), n-alkanoic diacids (C_2-C_{14}), unsaturated alkanoic acids ($C_{16:1}$-$C_{22:1}$), aromatic carboxylic acids and resin acids. The n-alkanes and n-alkanoic acids were found to be the most abundant target compounds.

1.6.2 Sources of Analytes Identified Previously

The sources of the compounds identified by Chen included biogenic sources, petrogenic sources and atmospheric transformation products. The sources of n-alkanes in the atmosphere were biogenic sources (e.g., epicuticular waxes and vascular plants)[75], and petrogenic sources (e.g., vehicle exhausts)[63]. The n-alkanoic acids were also found to have been derived from both biogenic and petrogenic sources. The biogenic sources include vegetative detritus and microorganisms[76], while vehicle exhausts also contain n-alkanoic acids[75]. n-Alkanoic diacids are believed to be the products of atmospheric

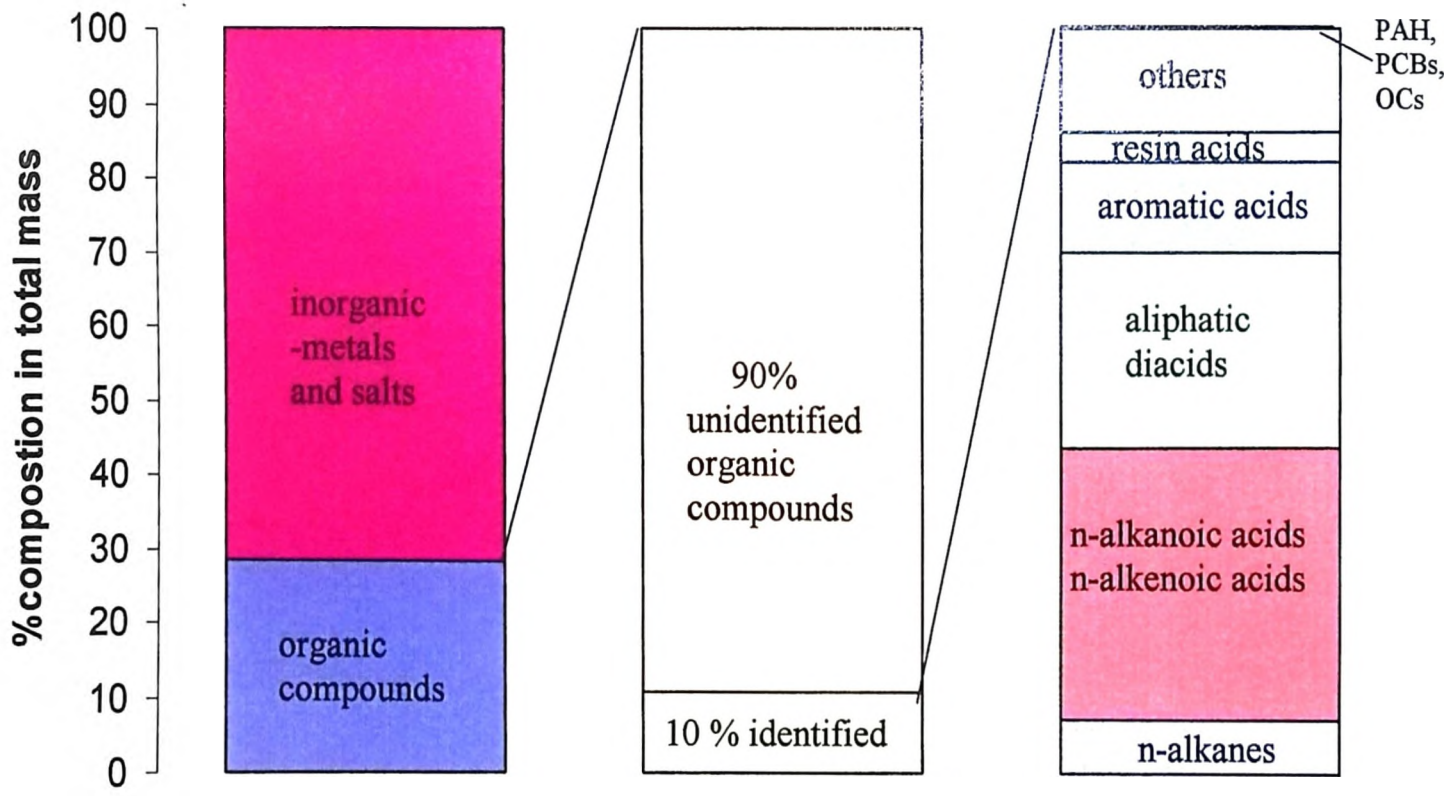


Figure 1-5. Chemical composition of 2.1 μm air particulate in the Los Angeles area (1982-2002) by Cass and Simoneit[63].

reactions[77,78], but have also been reported in meat cooking[79] and in the pyrolysis of biomass[80]. Aromatic (unsaturated) acids have been suggested to be atmospheric reaction products[84]. Resin acids are derived from wood combustion and are useful biomarkers for tracking wood smoke in the atmosphere[82].

1.7 Derivatization

While diazomethane readily converts carboxylic acids and phenols to their methyl derivatives, most hydroxyl-containing compounds remained unaffected. An alternative, more broad-spectrum derivatization method would be silylation. N-Methyl-N-trimethylsilyltrifluoroacetamide (MSTFA) is one of the more reactive silylation reagents[8]. Figure 1-6 depicts a general reaction scheme involving the derivatization of hydroxyl-containing compound using MSTFA. A major advantage of using MSTFA for silylation is that it forms a volatile and neutral by-product of N-methyltrifluoroacetamide (Figure 1.6), making it suitable for GC analysis. Due to its reactivity a drawback of using MSTFA is its susceptibility to hydrolysis.

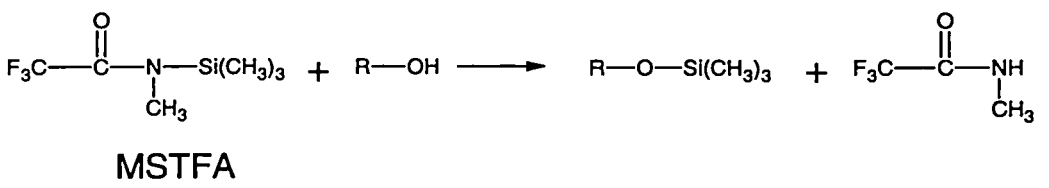


Figure 1-6. MSTFA readily converts hydroxyl-containing compounds to their trimethylsilyl derivatives.

Several recent reports have described using trimethylsilyl derivatization for the analysis of polar organic compounds in aerosol samples[3-5,22]. Some of the compounds identified were anhydrosugars (e.g., levoglucosan)[22], tetrols[37], and saccharides[19].

1.8 Other Sources of Window Film Material

Biomass burning is a source of a number of polar compounds in the atmosphere, including levoglucosan, which is formed from the pyrolysis of cellulose[22,23]. Simoneit et al. reported a number of saccharides in aerosols as being a result of re-suspension of soil (as well as the associated bacteria) from agricultural activities[19]. Airborne bacteria and spores have been reported to include polar compounds[83].

It is believed that the majority of the organic fraction found in aerosols are "Humic Like Substances" (HULIS)[87]. Humic substances are described as a complex class of refractory organic macromolecules, which result from the degradation of plants by microbes[84]. Havers et al. determined that the water-soluble organic carbon (WSOC) fraction of urban particulate resembled that of natural humic acids by UV/VIS, Fourier Transform infrared (FTIR) and by proton NMR (^{1}H-NMR) spectroscopy[84]. Decesari et al. were able to separate the WSOC fraction using ion-exchange chromatography and identified three generic classes: (1) neutral/basic compounds, (2) mono/di carboxylic acids, and (3) polycarboxylic acids. Using ^{1}H-NMR the chemical structures of the types of compounds found in each class were determined. The polycarboxylic acids were found to have an aromatic core with aliphatic chains containing –COOH, -CH_2OH, -$COCH_3$, and –CH_3 as terminal groups. These structures closely resemble terrestrial and

aquatic humic matter. Currently, new methods involving reversed-phase HPLC (RP-HPLC)[85] and capillary electrophoresis[86] are being developed in order to be able to further characterize the humic-like substances (HULIS).

1.9 Thesis Objectives

It has been shown that organic films present on impervious surfaces found in the environment play a critical role in the contaminant transport in urban areas and rural areas. The efficient removal of highly non-polar contaminants from the impervious surfaces by water (precipitation) was a completely counterintuitive observation. Thus, in order to be able to explain this phenomenon of non-selective wash-off the structures and properties of the chemical compounds that constitute the film must be investigated. The profiles of contaminants found in organic films were also shown to be similar to the profile of contaminants found in air particulate.

GC/MS was the workhorse instrument used in this thesis. Gas chromatography would provide good separation of these environmental samples and an electron impact mass spectrometer would provide mass spectra with fragment ions that can aid in the identification and quantification of analytes found in the organic films. Derivatization (e.g. trimethylsilylation) of polar compounds (e.g. sugars) was also used.

The main goals of this thesis are summarized as follows:

(1) To determine the structures of the chemical compounds that constitute the bulk of organic films on impervious surfaces found in urban and rural areas.

(2) To compare the chemical compositions of organic films to air particulate.

(3) To determine the reason for the non-selective wash-off of the various compounds contained within the organic film by simulated rain experiments.

2.0 EXPERIMENTAL

2.1 Chemicals

The following standards and reagents were purchased from Sigma-Aldrich (Milwaukee, WI, USA): arabinose, xylitol, levoglucosan, pinitol, L-quebrachitol, fructose, glucose, myo-inositol, sucrose, trehalose, maltitol, β-sitosterol, stigmastanol, 2-methyl-2-vinyloxirane, Diazald, carbitol, N-trimethylsilyl-N-methyltrifluoroacetamide (MSTFA), heptanoic acid (C_7), nonanoic acid (C_9), undecanoic acid (C_{11}), tridecanoic acid (C_{13}), pentadecanoic acid (C_{15}), nonadecanoic acid (C_{19}), tricosanoic acid (C_{23}), heptacosanoic acid (C_{27}), hentriacontanoic acid (C_{31}). Three deuterated PAH standards were purchased from Cambridge Isotope Labs Ltd. (Woburn, MA, USA): acenapthene-d_{10}, pyrene-d_{10} and perylene-d_{12}. O-Methylhydroxylamine hydrochloride was provided by Dr. E. A. Weretilnyk's lab (Biology, McMaster).

2.2 Gases & Solvents

High purity helium carrier gas (>99.999%) was purchased from VitalAire (Hamilton, ON, Canada). HPLC-grade solvents were purchased from Caledon Laboratories Ltd. (Georgetown, ON, Canada). Anhydrous pyridine was purchased from Sigma-Aldrich (Milwaukee, WI, USA).

2.3 Instrumentation

A Hewlett-Packard Model 5890 Series II gas chromatograph (Hewlett-Packard, Palo Alto, CA, USA) coupled to a Hewlett-Packard Model 5971A Mass Selective

Detector (Hewlett-Packard, Palo Alto, CA, USA) was used to analyze all samples by GC/MS. Analyses were performed in full scan mode using positive ion electron impact (EI^+) ionization with helium as the carrier gas. A DB-17ht capillary column (50% phenyl/50% methyl silicone, 30m length x 0.25mm i.d. x 0.15 μm film, J&W Scientific, Folsom, CA) was used for all sample analyses. A 5 m retention gap (deactivated fused silica, 5m x 0.53mm x 0.8mm, Chromatographic Specialties Inc, Brockville, ON) was placed on the front end of the column and connected to the DB-17ht column via a 2-way glass union (Chromatographic Specialties). Table 2-1 summarizes the column properties and temperature program used for the analyses.

Table 2-1. Column and instrument properties for GC/MS analysis.

Column Properties	
Column Type	J&W DB-17ht
Stationary Phase	50% phenyl, 50% methyl silicone
Column Length (m)	30
Column I.D. (mm)	0.25
Film Thickness (μm)	0.15
Carrier Gas	Helium
Flow Rate (mL/min)	0.958
Oven Temperature Program	
Initial Oven Temperature (°C)	50
Hold Time (min) at 50°C	5
Temperature Program Rate (°C/min)	5
Solvent Delay Time on MS (min)	13.5
Final Oven Temperature (°C)	300
Final Hold Time (min) at 300°C	5
Total Run Time (min)	60

2.4 Sample Collection

2.4.1 Collection of Window Film Samples

Sampling was performed by members of Dr. M.L. Diamond's research group at the University of Toronto. Untinted windows were sampled at various sites along a rural-suburban-urban gradient in the Toronto area in July 2000. The same windows were then sampled again in December 2000, March 2001, and July 2001. Samples were collected by scrubbing the surface of the window using dichloromethane-wetted Kimwipes (laboratory tissues) to within 10 cm of the window edge. Typically the samples represented 5-10 m^2 of window area at each location. All Kimwipes were cleaned prior to use by soaking them in HPLC grade dichloromethane for 2 minutes and allowing them to air dry in a fume hood. The cleaned Kimwipes were stored in dichloromethane-cleaned glass jars with Teflon-lined caps.

Further information about the samples used in this study is provided in Table 2-2.

2.4.2 Sample Extraction

Sample extractions were also performed at the University of Toronto by Dr. M.L. Diamond's research group. The samples were first extracted in a Soxhlet apparatus with 180 mL of dichloromethane at a cycle rate of 20 cycles per hour for 12 hours. A second extraction using 180 mL of methanol for 12 hours was also done. The dichloromethane

Table 2-2. Sampling site locations and descriptions.

Code	Location of Sample Collection	Sampling Date		Site Description			
		Mar-01		Location Character	Building Function	Outdoor Environment	Indoor Activity
		Outdoor	Indoor				
EB (rural office)	Egbert	Y	Y	rural	office/laboratory building	in an agricultural area, surrounded by monotyledonous plants	food handling involved
DW (suburban office)	Downsview	Y	Y	suburban	office building	on an arterial road, surrounded by grass areas and deciduous trees	office
RS (urban residence)	Downtown, Toronto	Y	Y	urban	family residences, composite of five 100-year old houses	surrounded by grass areas and deciduous trees	cooking involved
SR (urban office)	South Riverdale	Y	Y	urban	office and meeting room	on major street with heavy traffic	N/A
PHW (urban laboratory)	Pharmacy Building West, University of Toronto	Y	Y	urban	laboratory building	surrounded by grass areas and deciduous trees	conducting research involving lipids and fatty acids
JR (urban restaurant)	Downtown, Toronto	Y	Y	urban	restaurant	on an arterial road, surrounded by grass areas and deciduous trees	drinking, cigarette smoking and cooking involved

and methanol extracts were concentrated separately to approximately 1 mL at 23°C under N_2 using a Zymark Turbovap II concentrator. The extracts were then passed through separate columns packed with 3-5 g of anhydrous Na_2SO_4. The columns were eluted with either dichloromethane or methanol (3 x 1 mL) and the collected eluate was made up to a final volume of 10 mL in a volumetric flask. Dichloromethane extracts were divided into three aliquots (4 mL, 4 mL, 2mL), while the methanol extracts were portioned into two aliquots (5 mL, 5 mL). Samples were stored at -18°C in glass vials sealed with Teflon-lined caps.

2.4.3 Determinations of Film Masses, Organic Matter and Extractable Materials

Diamond's research group also handled the determinations of film masses, organic matter and film thickness calculations. A gravimetric method was used to determine the total mass of material collected from the various windows. Kimwipes were dried for 24 hours in the presence of silica gel, before and after sampling, and then weighed. Total carbon (TC, elemental and organic) was measured using a Perkin Elmer Model 240-XA Elemental Analyzer at the Freshwater Institute (Winnipeg, Manitoba). Organic matter (OM) was determined by multiplying the TC values by 1.5, a common factor for the conversion of carbon mass to average organic mass. Using a density of 0.826 g/cm^3 (density of n-octanol) the organic film thickness was calculated from the masses of organic matter.

Masses of extractable material masses were determined at McMaster University by a previous member of our research group (R. Chen). Aliquots of the dichloromethane

extract (100-200 μL) or the methanol extract (400 μL) were placed on a pre-dried and pre-weighed planchette. The solvent was allowed to evaporate and then samples were dried in a dessicator over P_2O_5 for 24 hours. A Mettler balance (Type M5SA), which is accurate to the microgram range, was used to determine the masses. The net masses ranged from 20 μg to 100 μg for dichloromethane extracts and 100 μg to 4000 μg for methanol extracts.

2.4.4 Previous Handling of Samples

The Diamond group provided portions of the dichloromethane extracts (about 2 mL) and methanol extracts (5 mL) of the window films to our group. Prior to this work the samples were handled as follows: volumes of the dichloromethane extracts were measured prior to use and volume losses were made up with dichloromethane. Methanol extracts were blown down to about 0.5 mL and then transferred to 2 mL volumetric flasks. The vials were rinsed with methanol (3 x 300 μL) and each washing was transferred to the 2 mL volumetric flask before diluting to volume (2 mL).

2.5 Procedures for the Preparation of Standards

2.5.1 Preparation of Internal Standards

Three deuterated PAH standards were used as internal standards in the experiments: acenaphthene-d_{10}, pyrene-d_{10}, and perylene-d_{12}. Each standard was weighed individually using a six-place balance and placed into a 10 mL volumetric flask. The volume was made up using toluene resulting in concentrations of acenapthene-d_{10},

pyrene-d_{10}, and perylene-d_{12} of 222 ng/μL, 177 ng/μL and 172 ng/μL, respectively. An aliquot of the internal standard was then used in the preparation of the retention index standard (Section 2.5.2).

2.5.2 Preparation of Retention Index Standard

A retention index (RI) approach was used to aid in the identification of compounds found in the window films. In this work saturated fatty acids were derivatized as their trimethylsilyl esters using MSTFA and used as the retention index standards. Nine odd-carbon saturated fatty acids ranging from C_7 to C_{31} were assigned the following retention index values: heptanoic acid TMS ester (C_7) = 700; nonanoic acid TMS ester (C_9) = 900; undecanoic acid TMS ester (C_{11}) = 1100; tridecanoic acid TMS ester (C_{13}) = 1300; pentadecanoic acid TMS ester (C_{15}) = 1500; nonadecanoic acid TMS ester (C_{19}) = 1900; tricosanoic acid TMS ester (C_{23}) = 2300; heptacosanoic acid TMS ester (C_{27}) = 2700; and hentriacontanoic acid TMS ester (C_{31}) = 3100.

A stock solution of the retention index standards was prepared according to a procedure developed by a previous member of our group, Julia Jia[9]. The procedure is illustrated in Figure 2-1a and a chromatogram of the fatty acid TMS esters is shown in Figure 2-1b. From the stock solution a 10 μL aliquot of the fatty acid standard solution was taken and placed into a 1.5 mL vial with a septum cap and blown to dryness using N_2. A 12 μL aliquot of an internal standard solution was then added to the vial and the final volume was made up to 350 μL by adding 35 μL of MSTFA and 303 μL of toluene so that MSTFA would constitute about 10% of the solution. The vial was stored in the

refrigerator until it was needed. Table 2-3 summarizes the concentrations of the standards used.

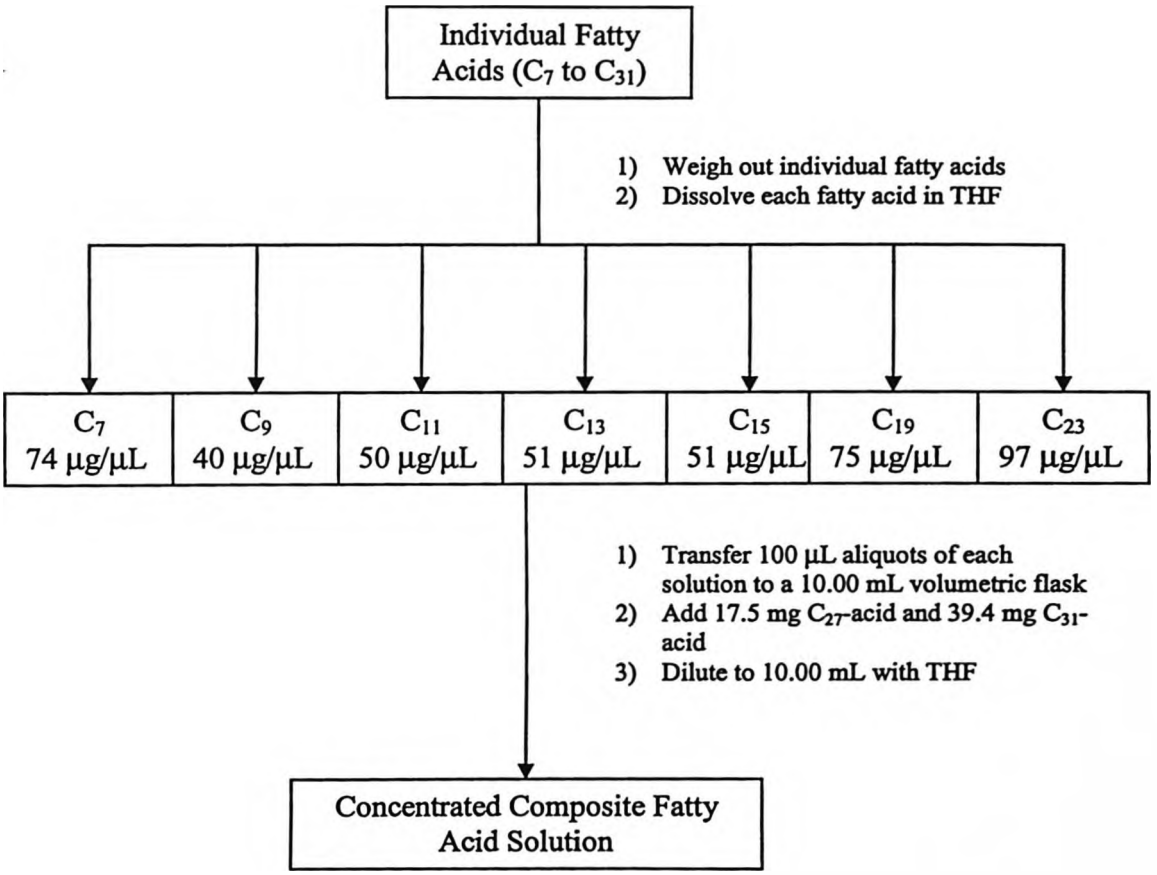


Figure 2-1a. Preparation of Fatty Acid Retention Index Standard Solution.

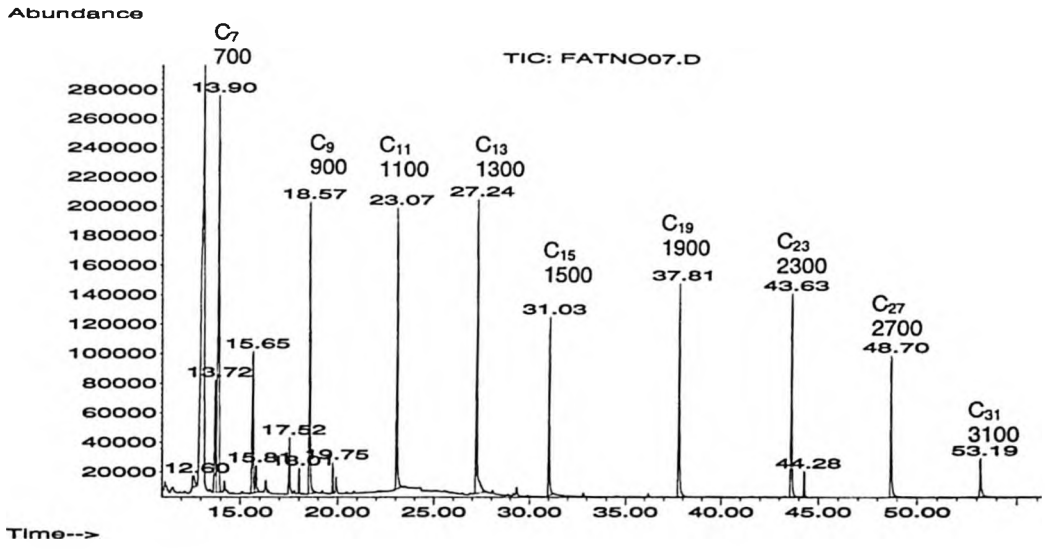


Figure 2-1b. Fatty Acid (TMS) Esters Retention Index Standard (C_9-C_{31})

Table 2-3. Concentrations of Fatty Acids and Internal Standards.

Fatty Acid Standards	Stock Concentration of Fatty Acid (ng/μL)	Volume Taken (μL)	Concentration in Mixture (ng/μL) Final Volume = 350 μL
Heptanoic Acid (C_7)	740	10	21.1
Nonanoic Acid (C_9)	400	10	11.4
Undecanoic Acid (C_{11})	498	10	14.2
Tridecanoic Acid (C_{13})	510	10	14.6
Pentadecanoic Acid (C_{15})	506	10	14.7
Nonadecanoic Acid (C_{19})	749	10	21.4
Tricosanoic Acid (C_{23})	973	10	27.8
Heptacosanoic Acid (C_{27})	1750	10	50.0
Hentriacontanoic Acid (C_{31})	3940	10	113
Internal Standards	**Stock Concentration of Internal Standard (ng/μL)**	**Volume Taken (μL)**	**Concentration in Mixture (ng/μL) Final Volume = 350 μL**
Acenaphthene-d_{10}	222	12	7.59
Pyrene-d_{10}	177	12	6.05
Perylene-d_{12}	172	12	5.90

2.6 Calculations

2.6.1 Determination of Retention Index Values

The retention index value of each peak was calculated using the following formula:

$$\text{Retention Index (RI)} = 100y + 100(z-y) \times [(t_r(x)-t_r(y))/(t_r(z)-t_r(y))]$$

where x is the peak of interest, y is the carbon number of the retention index standard that elutes prior to the peak of interest, and z is the carbon number of the retention index standard that elutes after the peak of interest. The retention time of the peak of interest is $t_r(x)$, while $t_r(y)$ and $t_r(z)$ are the retention times of retention index standards that have carbon numbers y and z.

2.6.2 Determination of Relative Response Factors

A solution containing various sugars and sugar alcohols was prepared from standards that had been previously weighed and stored at -20°C. Prior to derivatization, each standard was thawed completely and aliquots of each solution were combined into a single glass vial. The standard mixture was derivatized using a similar procedure to that used for the window films samples (section 2.7.1). Toluene was used to dilute the sample several times and each dilution was analyzed by GC/MS in full scan mode. If two or more derivatives were produced, each derivative was assumed to have an identical response factor to the others; therefore the total response was equal to the sum of the peak areas of all the derivative peaks. The standards and the relative response factors of their derivatives are shown in Table 2-4.

The peak area of each derivative was plotted against the mass of each underivatized standard injected (ng). A linear least squares line of best fit was drawn through the data points using Excel; the slopes and R^2 values were determined. The same procedure was done for the PAH internal standards added into the mixture. The ratio of the slope of the derivative line of best fit to the slope of the PAH line of best fit (in the same injection) gave the relative response factor. Response factors were also calculated using mass chromatograms. The ions used for quantitation (Table 2-4) were chosen because of their sensitivity and relatively low interference with matrices.

A solution containing the fatty acids C_{16}, C_{18}, and C_{20} was also prepared so that they could be converted to their methyl esters. Aliquots from stock solutions of each fatty acid were placed into a 10 mL volumetric flask and the volume was made up using dichloromethane. A volume of 10 μL was then taken from the diluted mixture and derivatized in a manner similar to the procedure found in Section 2.7.2. The relative response factors were determined using the following formula:

$$\text{Relative Response Factor (RRF)} = (A_{\text{cal std}}/M_{\text{cal std}})/(A_{IS}/M_{IS})$$

where $A_{\text{cal std}}$ is the area of the calibration standard, $M_{\text{cal std}}$ is the mass (ng) of the calibration standard injected, A_{IS} is the area of the internal standard, and M_{IS} is the mass (ng) of the internal standard injected.

Table 2-4. Relative Response Factors of Selected Standards and Detection Limits.

Standard	Derivatized Standard	$R^{2[e]}$	Relative Contribution to Derivatives (%)[a]	Quantitating Ion	Detection Limits (ng/µL)	RRF[a,b]	STDEV[c] of RRF	RSD[d] of RRF
C_5-tetrol	C_5-tetrol-$(TMS)_4$	n/a	100	219	0.1	0.28	0.02	6%
C_5-tetrol	C_5-tetrol-$(TMS)_4$	n/a	100	219	0.1	0.25	0.01	5%
Arabinose	Arabinose MeOX1-$(TMS)_4$	0.997	80 ± 2	103	0.1	0.78	0.07	9%
	Arabinose MeOX2-$(TMS)_5$		20 ± 2					
Xylitol	Xylitol-$(TMS)_5$	0.997	100	217	0.1	1.08	0.11	10%
Acenapthene-d_{10}	-	0.997	100	164	-	0.66	0.03	4%
Levoglucosan	Levoglucosan-$(TMS)_3$	0.998	100	217	0.1	0.50	0.04	8%
Pinitol	Pinitol-$(TMS)_5$	0.999	100	260	0.1	0.39	0.03	7%
L-Quebrachitol	L-Quebrachitol-$(TMS)_5$	0.995	100	217	0.1	0.44	0.05	11%
Mannitol	Mannitol-$(TMS)_6$	n/a	100	319	0.1	2.19	n/a	n/a
Fructose	Fructose MeOX1-$(TMS)_5$	0.998	63 ± 2	103	0.1	0.71	0.08	12%
	Fructose MeOX2-$(TMS)_6$		37 ± 2					
Glucose	Glucose MeOX1-$(TMS)_5$	0.998	82 ± 2	205	0.1	0.67	0.08	12%
	Glucose MeOX2-$(TMS)_6$		18 ± 2					
Myo-Inositol	Myo-Inositol-$(TMS)_6$	0.998	100	217	0.1	1.03	0.08	8%
Pyrene-d_{10}	-	0.998	100	212	-	1.00	-	-
Sucrose	Sucrose-$(TMS)_8$	0.995	100	361	0.2	0.73	0.08	10%
Trehalose	Trehalose-$(TMS)_8$	0.993	100	361	0.2	1.48	0.13	9%
Maltitol	Maltitol-$(TMS)_9$	0.998	100	204	0.3	0.61	0.06	9%
Stigmastanol	Stigmastanol-TMS	n/a	100	215	0.3	0.05	n/a	n/a
β-Sitosterol	β-Sitosterol-TMS	n/a	100	129	0.3	0.04	n/a	n/a
Perylene-d_{12}	-	0.995	100	264	-	0.59	0.03	4%
Hexadecanoic Acid	Hexadecanoic Acid Methyl Ester	n/a	100	74		0.57	0.09	15%
Octadecanoic Acid	Octadecanoic Acid Methyl Ester	n/a	100	74		0.79	0.10	13%
Eicosanoic Acid	Eicosanoic Acid Methyl Ester	n/a	100	74		0.69	0.12	17%

a: Values are based on the average of 3 separate experiments (stigmastanol, β-sitosterol are based on a single experiment)
b: RRF = Relative Response Factor relative to Pyrene-d_{10} (C_5-tetrols, mannitol, stigmastanol, b-sitosterol RRFs were calculated using the formula in Section 2.6.2)
c: STDEV = Standard Deviation
d: RSD = Relative Standard Deviation
e: R^2 = Square of the correlation coefficient for linear least squares best fit

2.6.3 Quantitation

Quantitation of the analytes was achieved by comparing the peak areas of quantitating ion in the mass chromatogram of the analyte to the peak area of the quantitating ion in the mass chromatogram of an internal standard added. The following formula was used to calculate the mass of a given analyte:

$$M_{analyte} = (A_{analyte} \times M_{IS})/(RRF \times A_{IS})$$

where $M_{analyte}$ is the mass (ng) of the analyte injected, and $A_{analyte}$ is the peak area of the quantitating ion of the analyte. Quantitation of the various analytes was performed following a procedure involving oximation then trimethylsilylation (Section 2.7.1).

In order to determine the amount of the original sample remaining, the following rather convoluted analysis procedure was developed. The masses per unit area (ng/m^2) of the C_{16}-methyl ester, C_{18}-methyl ester, and C_{20}-methyl ester in the dichloromethane and methanol extracts had been determined previously as described by R. Chen[1] (Appendix 4). The C_{16}, C_{18} and C_{20} fatty acids (determined as their methyl esters) were found to be predominant in the methanol extracts of the window film samples analyzed by R. Chen. By using the mass (ng) of the methyl esters found in the methanol extract and by knowing the loadings of the fatty acids (ng/m^2 values Appendix 4) the number of m^2 of window area injected could be determined. Thus, to get the number of m^2 of sample injected, 5 μL aliquots of methanol window film extracts were derivatized with CH_2N_2 to give methyl esters followed by treatment with MSTFA. The values of the C_{16}, C_{18} and C_{20} fatty acid methyl esters were then used to determine the mass per unit area of these analytes.

2.7 Procedure for the Analysis of Window Film Samples

2.7.1 Oximation/Trimethylsilylation Procedure

A 5 μL aliquot of a methanol extract of a window film sample was added to a GC-vial (Chromatographic Specialties, Q-Sert Vial, 250 uL), followed by a solution of 9-anthracenemethanol (25.5 ng/μL in DCM, 10 μL). The solvent was evaporated to dryness using a gentle stream of N_2 (g). A solution of $MeONH_2 \bullet HCl$ in pyridine (20 mg/mL, 20 μL) was added to the dried extract and allowed to react at 37°C for 90 minutes (an additional 10 minutes was added to allow the mixture to reach 37°C). Then, neat MSTFA (20 μL) was added and the reaction heated for an additional 30 minutes (+10 minutes) at 37°C. The reaction mixture was blown down to dryness using a gentle stream of N_2 (g). When the bulk of the derivatizing reagents had evaporated, the GC-vial was flicked with a finger so that the remaining precipitate was spread along the sides of the vial rather than all clumped at the bottom of the vial. A solution (10 μL) of the retention index standard containing fatty acid TMS esters and PAH internal standards in a toluene solution containing MSTFA (10% by volume) was added to the dried derivatized extract. A portion of the resulting solution (1 μL) was injected onto the GC/MS.

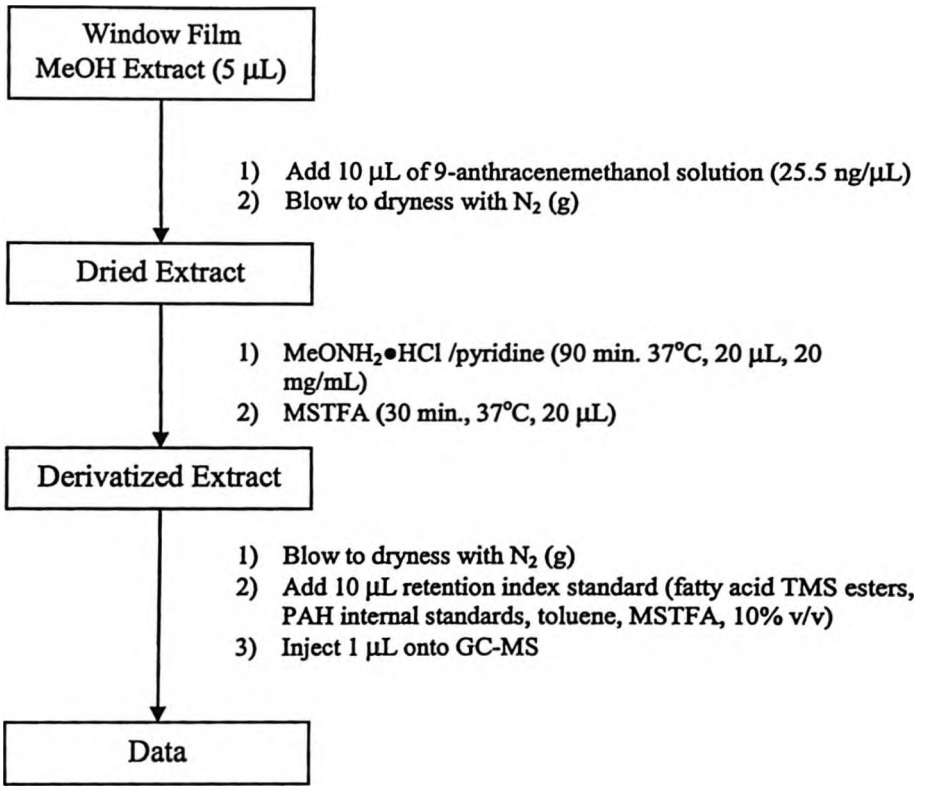


Figure 2-2. Oximation/trimethylsilylation Procedure for the Analysis of Window Film Samples.

2.7.2 Methylation/Trimethylsilylation Procedure

Methylation was performed using diazomethane (CH_2N_2) generated from Diazald (N-methyl-N-nitroso-p-toluenesulfonamide) in a small scale reactor[1].

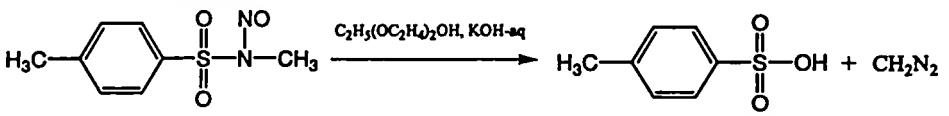


Figure 2-3. Reaction for the Generation of CH_2N_2 from Diazald.

The reaction was performed in an Aldrich Diazomethane Generator. Dichloromethane (5 mL) was placed into the outer tube of the generator. Diazald (0.3-0.4 g) was placed into the inner tube followed by 1 mL of diethyl ether, 1 mL of carbitol and a micro magnetic stirrer. The inner tube was capped with a screw cap containing a Teflon-silicone septum and was then placed into the outer tube and clamped tightly. The entire assembly was placed into an ice-water bath so that the dichloromethane in the outer tube was totally immersed, while the reactants in the inner tube remained above the bath level. A solution of KOH (37%, 1.5 mL) was added to initiate diazomethane generation by adding the basic solution in a dropwise manner through the Teflon-silicone septum using a plastic syringe with a narrow needle gauge. Aluminum foil was used to wrap around the generator so as to exclude any light. The reaction was stirred and allowed to proceed for an hour. The resulting diazomethane solution in the outer vessel was used immediately for methylation reactions.

For the silylation reaction a 5 μL aliquot of the methanol extract of the window film samples and 10 μL of a 9-anthracenemethanol solution (25.5 ng/μL) were placed directly into a GC-vial and blown to dryness using N_2 (g). To the dried extract was added a solution of CH_2N_2 (20 μL) (prepared as in Section 2.7.2). The GC-vial was covered with aluminum foil and the reaction allowed to proceed for 30 minutes with occasional shaking at room temperature. Excess CH_2N_2 was removed in the fumehood using a stream of N_2 (g). Pyridine (20 μL) followed by MSTFA (20 μL) was added to the dried methylated extract and allowed to react for 30 minutes (+10 minutes) at 37°C. The reaction mixture was blown to dryness; again ensuring that the GC-vial was flicked so

that any precipitate coats the sides of the vial rather than the bottom. A sample of the retention index standard (10 μL) was added and 1 μL was injected on the GC/MS.

2.8 Monitoring the GC Column Performance

Given the dirty nature of the window film samples and the fact that there was no clean-up step prior to derivatization, the performance of the GC column tended to deteriorate rather quickly. Each day prior to any injections a 200 pg/μL PAH calibration standard was run to check column performance. The PAH standard was run using a temperature program starting at 90°C with the temperature increasing at a rate of 8°C/min. up to a final temperature of 300°C. The temperature was held at 300°C for 25 minutes. Peak widths of six 252 amu PAH (benoz[b]fluoranthene, benzo[k]fluoranthene, benzo[j]fluoranthene, benzo[e]pyrene, benzo[a]pyrene and pyrene) were used to assess column performance. Typically, peak widths below 0.045 minutes indicated that the column was performing well. In general, 2-3 injections of the window film samples could be injected before the column performance became unacceptable. Normally, cutting 0.5-1 m of the retention gap would restore the performance of the column. A PAH calibration standard solution was injected after cutting the retention gap to ensure that the column performance had been restored.

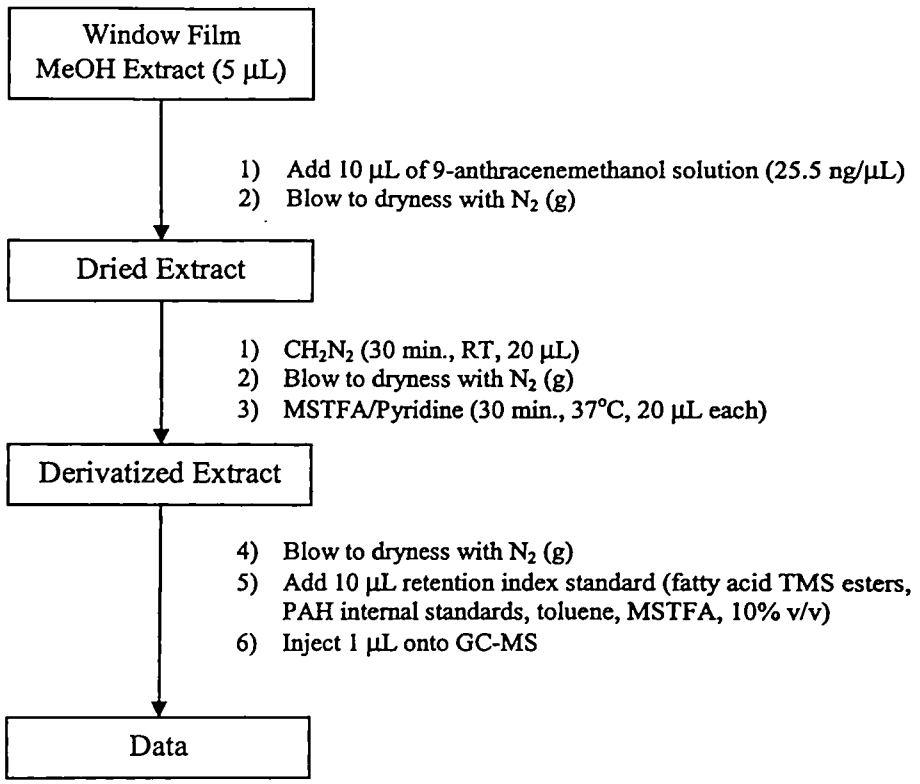


Figure 2-4. Methylation/trimethylsilylation Procedure for the Analysis of Window Films.

2.9 Tetrol Synthesis

The compounds 2-methylthreitol and 2-methylerythritol were synthesized from 2-methyl-2-vinyloxirane using a peroxidation/hydrolysis procedure with performic acid[11,12].

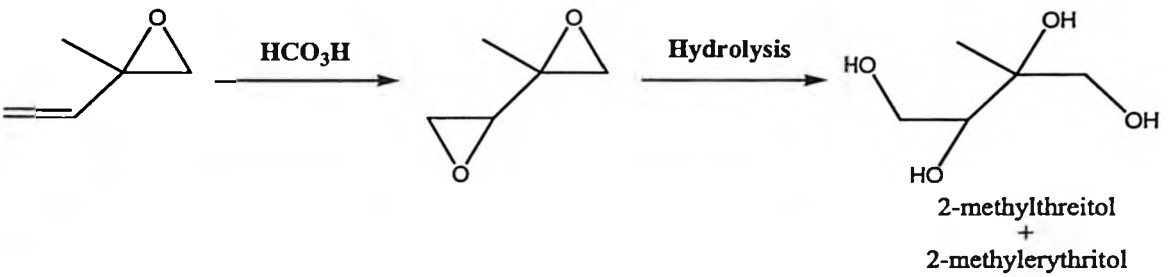


Figure 2-5. Synthesis of 2-methylthreitol and 2-methylerythritol from 2-methyl-2-vinyloxirane.

Formic acid (HCOOH, 21 g, 90%), 30% hydrogen peroxide (H_2O_2, 2.6 g), and 2-methyl-2-vinyloxirane (1.68 g) were placed in a 100 mL round bottom flask. Two immiscible layers resulted and were shaken together briefly. The mixture was then placed in a water bath at 65-70°C for 2 hours. The reaction mixture was allowed to cool and was reduced in volume to approximately 5 mL using a rotary evaporator. Then 20% aqueous NaOH (8 mL) was added and the mixture heated to 80-95°C for 45 minutes. After cooling to room temperature 6N HCl was added to neutralize the solution. The mixture had a yellow colour and was reduced in volume using a rotary evaporator down to a few milliliters, transferred to a 25 mL round bottom flask and then evaporated to dryness. A wet residue of NaCl and the products remained in the flask. The flask was dried at 0.02 mm at 25°C before it was distilled under vacuum using a Buchi Kugelrohr oven (Buchi GKR-50). The boiling point of the product was not known but was estimated to be somewhat less than that for 1,2,3,4-butanetetrol (330.7°C[13] at atmospheric

pressure). The vacuum during the Kugelrohr distillation was 0.1 mm Hg which corresponds to a boiling point of the tetrol around 130-140°C. The temperature on the Kugelrohr was set to 150°C and the distillation allowed to proceed. A clear viscous liquid (6.6 mg) collected in the distillate reservoir. Characterization of the tetrols was done by obtaining ^{1}H-NMR and ^{13}C-NMR spectra (Bruker 600MHz NMR Spectrometer) and a probe mass spectrum on a GC-TOF (Micromass GCT) (see data in Appendix 3).

3.0 ANALYTICAL METHOD DEVELOPMENT

3.1 Background to Optimizing a Small-scale Analytical Method

The samples analyzed in this study were provided by the M.L. Diamond research group at the University of Toronto (department of Geography) as part of a joint research project. All sample collections, extractions and film mass measurements were performed in Diamond's research group as part of this project. At McMaster University a previous member of our research group (R. Chen) had developed an analytical method for the analysis of 85 target analytes involving diazomethane treatment of the samples followed by GC/MS analysis for the determination of fatty acids, diacids, aromatic acids and resin acids. During the course of her work almost all of the window film extracts had been used; most of the dichloromethane extracts had been used up completely, but there were very small quantities remaining of most MeOH extracts. Due to these severe sample limitations an analytical method had to be developed such that these analyses could be performed reproducibly on a small scale.

3.1.1 Trimethylsilyl Derivatization

Several reports had shown that polar hydroxyl-containing compounds were present in aerosol extracts[2-6], including various sugars[7]. At the time this work began another graduate student (J. Jia) was in the process of developing a comprehensive method for the analysis of polar cell metabolites, including sugars, based on a published procedure[9]. This method was developed to be performed on a small scale. All hydroxyl-containing compounds were converted into their trimethylsilyl (TMS) derivatives using

the powerful silylation reagent, MSTFA. In order to determine whether a silylation approach would be a useful derivatization method in this work, a methanol extract of a window film sample was treated with MSTFA since very little of any of the corresponding DCM extracts remained. For this first attempt a 100 µL aliquot of a MeOH extract was blown to dryness in a Reactivial and treated with dry pyridine and MSTFA (30 µL each) for 30 minutes at 37°C. A portion of the derivatized mixture (10 µL) was then diluted ten-fold with ethyl acetate and an aliquot (1 µL) submitted to GC/MS analysis. Figure 3-1 shows the full scan total ion chromatogram from this first experiment.

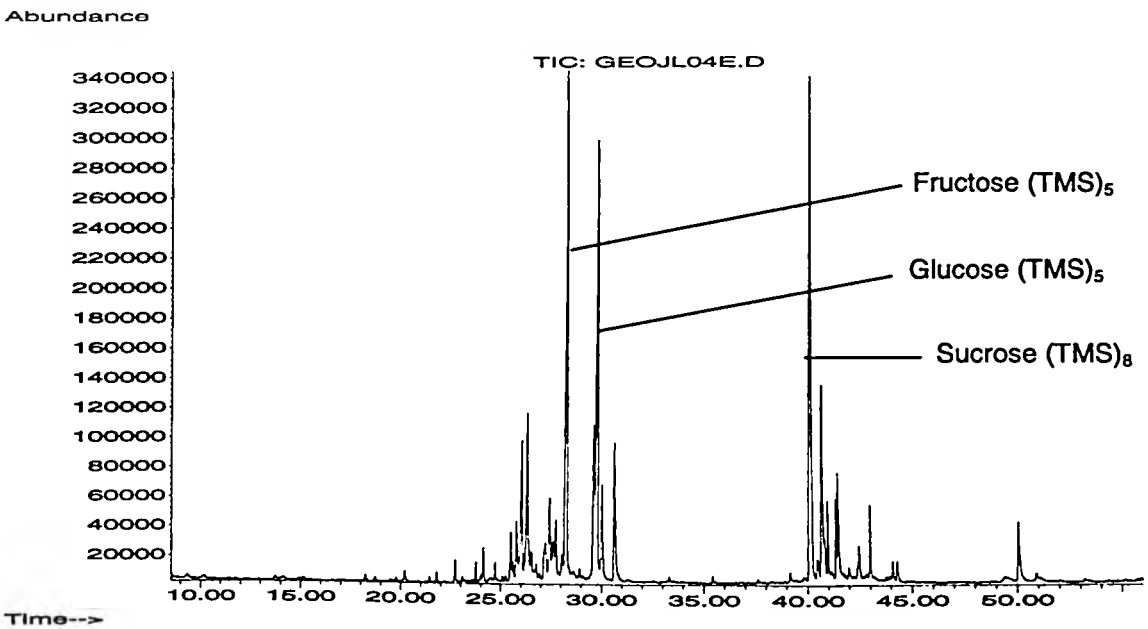


Figure 3-1. GC/MS total ion chromatogram of MSTFA-derivatized window film extract.

The chromatogram showed numerous well-resolved peaks with a surprisingly clean baseline. By using the NIST 2002 mass spectral database, tentative identifications of the major peaks were found to correspond to TMS derivatives of fructose, glucose, and sucrose.

3.1.2 Methoximation Derivatization Prior to Silylation

Much of the method development in this project borrowed heavily from the work of J. Jia who was developing methods for profiling polar metabolites in the plant, *Thellungiella salsuginea.* Among the metabolites she identified were amino acids, monosaccharides, disaccharides and sugar alcohols[9]. The procedure she developed was adapted from a method reported by Fiehn et al.[8], wherein samples were treated with O-methylhydroxylamine hydrochloride in pyridine (37°C, 90 min.) followed by trimethylsilylation with MSTFA (37°C, 90 min.).

Carbonyl-containing sugars such as fructose and glucose can form a variety of cyclic and open-chain products when subjected only to TMS derivatization[10]. By using hydroxylamine (or alkoxyamine) hydrochlorides, all aldehydes and ketones are converted to their respective E- and Z-oxime products thereby precluding the cyclization of any reducing sugars[10]. Subsequent derivatization with MSTFA results in the formation of volatile TMS derivatives of these E- and Z-isomers. For example, the reaction of glucose with methoxylamine hydrochloride in pyridine results in the formation of the E- and Z-glucose MeOX derivative in a ratio of 83:17 (Figure 3-2). The subsequent reaction with MSTFA converts these oximes to their penta-TMS derivatives.

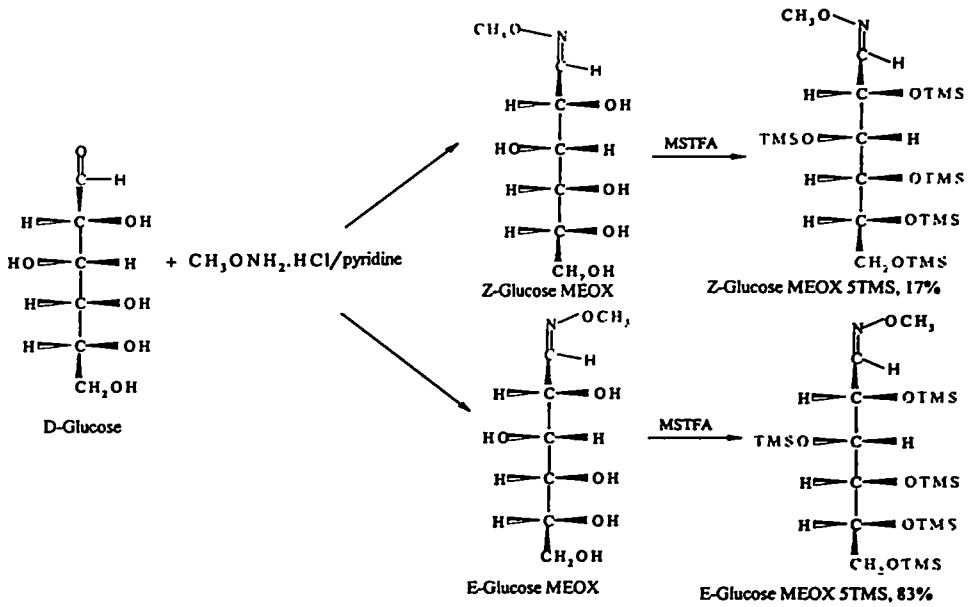


Figure 3-2. Two-step derivatization of glucose using O-methylhydroxylamine hydrochloride followed by MSTFA.

Figure 3-3 shows the difference that the methoximation reaction prior to silylation makes on the resulting chromatograms in the analysis of glucose. In Figure 3-3a the reaction of glucose with MSTFA results in the formation of four peaks (28.14 min., 28.33 min., 29.16 min. and 30.64 min.), while in Figure 3-3b the reaction of glucose with methoxylamine followed by MSTFA results in only two glucose derivative peaks (28.00 min and 28.20 min.) in a 85:15 ratio.

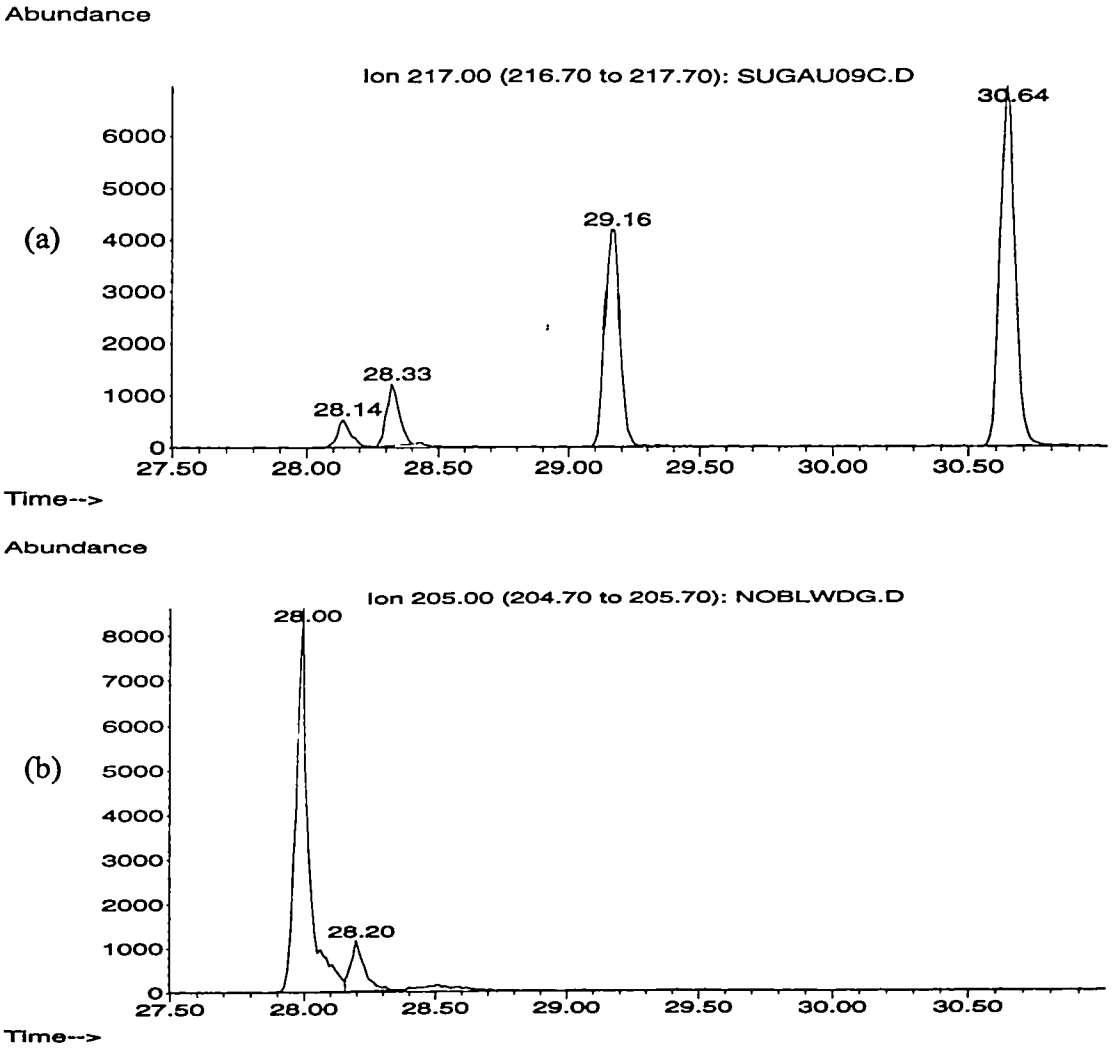


Figure 3-3. GC/MS mass chromatograms of glucose derivatives using (a) Derivatization with MSTFA only. (b) Derivatization with $MeONH_2 \cdot HCl$/pyridine followed by MSTFA.

3.1.3 GC/MS Analysis of Derivatization Reaction Mixtures

In order to be able to perform analyses on small amounts of window film extract samples the volume of MeOH window film extract used needed to be kept as small as possible so that the samples would not be depleted. The size of the aliquot of film extract was reduced to 5 μL. The following derivatization procedure was attempted: A 5 μL sample of the film extract was placed directly into a GC vial (instead of a Reactivial) and then blown to dryness in with a stream of N_2 (g), derivatized with 5 μL of $MeONH_2 \bullet HCl$/pyridine (20 mg/mL, 37°C, 90 min.), followed by 5 μL of MSTFA (37°C, 30 min.). A 1 μL aliquot of the resulting sample was injected neat directly onto the GC column. The resulting chromatogram (Figure 3-4) shows that the derivatization appeared to be working; however there was a major peak at about 10 minutes of the chromatogram, which was shown to be N-methyltrifluoroacetamide (Figure 3-5), a byproduct of the MSTFA reaction.

Since pyridine, MSTFA and N-methyltrifluoroacetamide are reasonably volatile, it was proposed to blow down the reaction mixture to reduce the levels of these substances and then take up the residue to analyze the "non-volatiles". The derivatization procedure was performed again as above on another aliquot of the window film sample; the reaction solution was blown down to dryness with N_2 (g) and taken back up in a toluene/MSTFA solution (80:20). MSTFA was added to the toluene due to the ability of TMS derivatives to undergo rapid hydrolysis in the presence of traces of water. Figure 3-6 shows a comparison of chromatograms from the reaction blanks from these two procedures; it is evident that blowing down the mixture after derivatization reduces the

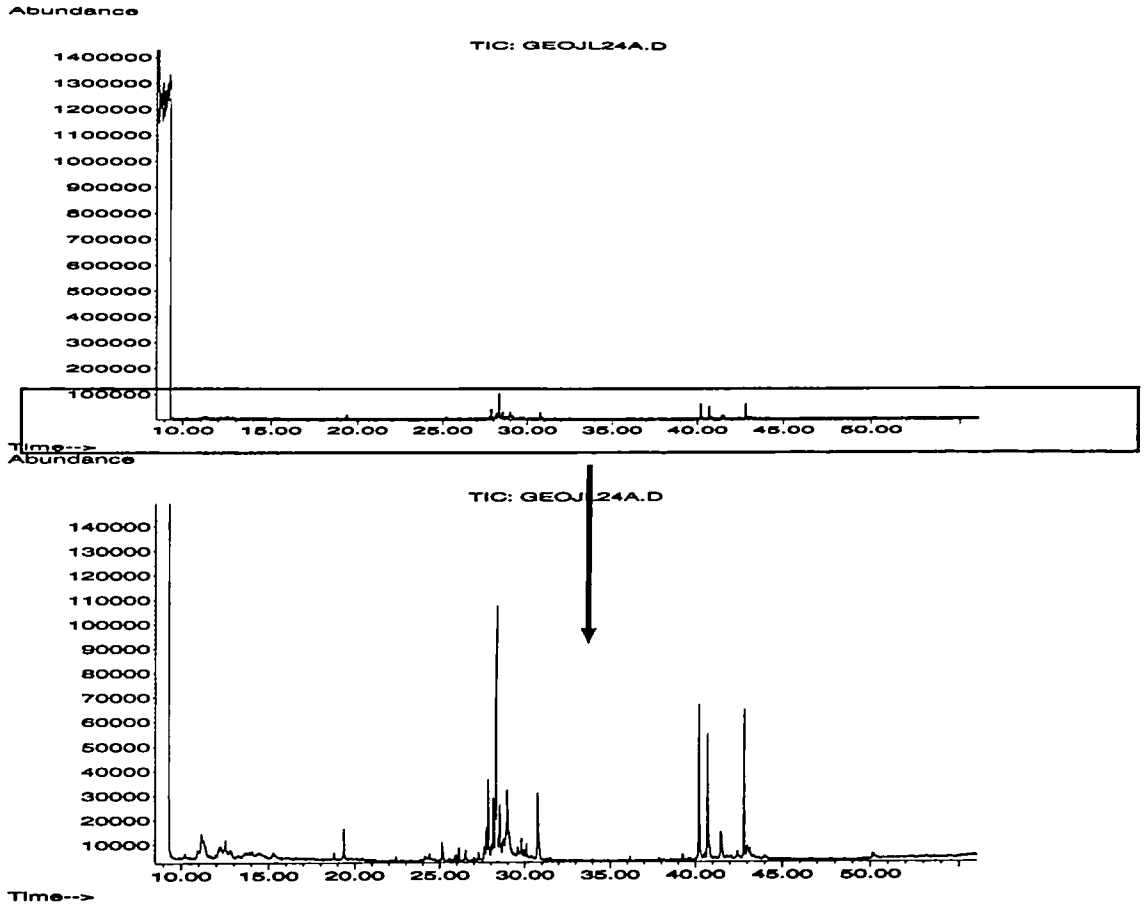


Figure 3-4. Neat injection of a window film extract and derivatizing reagents ($MeONH_2$•HCl/pyridine and MSTFA).

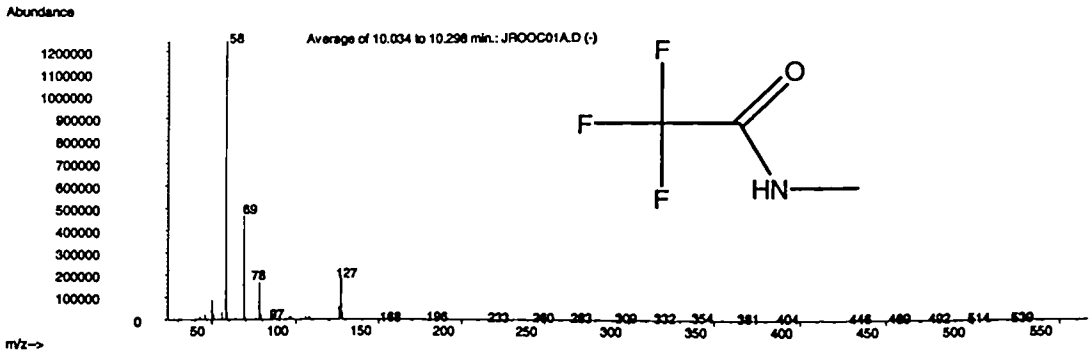


Figure 3-5. Mass spectrum of N-Methyltrifluoroacetamide.

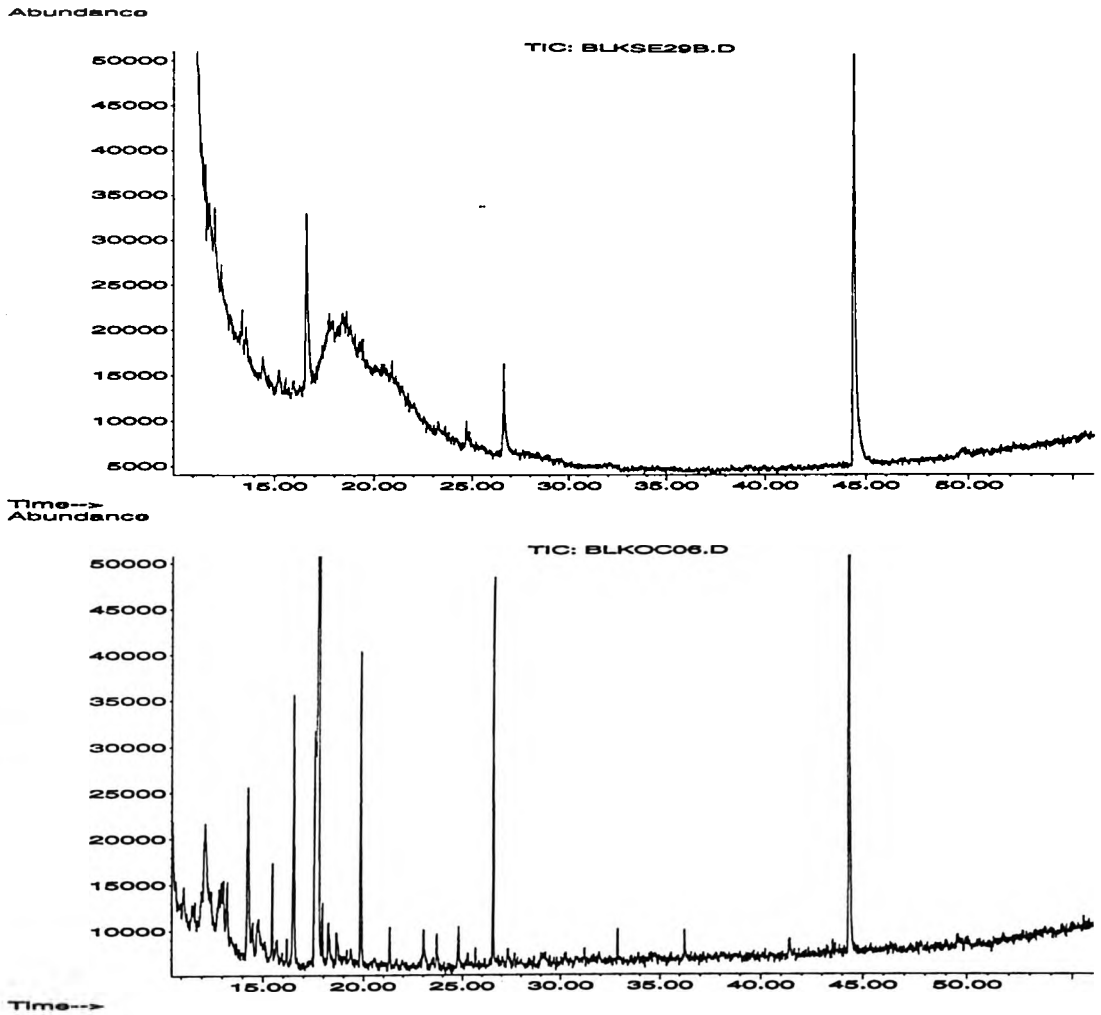


Figure 3-6. (a) Neat injection of reaction blank consisting of $MeONH_2 \cdot HCl$/pyridine and MSTFA. (b) Injection of reaction blank following blow down and dissolution in a toluene/MSTFA solution (80:20).

background considerably. This blow down step was incorporated into the sample preparation procedure for the analysis of window films. Additionally, the solvent delay of the temperature program was set to 13 minutes to exclude any interference due to residual N-methyltrifluoroacetamide.

3.1.4 Evaluation of O-Methylhydroxylamine Hydrochloride Concentrations

In an attempt to reduce some of the GC/MS background, the concentration of $MeONH_2 \bullet HCl$/pyridine was varied from 20 mg/mL to 2 mg/mL. A solution of hydroxyl-containing standards that included ribitol, pinitol, glucose, sucrose and melibinose was used to evaluate these reactions. As the concentration of O-methylhydroxylamine hydrochloride was reduced, analysis of the chromatograms showed that the reaction of glucose was no longer going to completion; glucose is the only compound in this mixture of standards that would react in the $MeONH_2 \bullet HCl$/pyridine reaction. Figure 3-7 highlights the region of the chromatogram where glucose derivatives elute (28.02 and 28.22 min.). Figure 3-7 shows that the 2 mg/mL reaction resulted in decreased levels of the desired derivatives at 28.02 min. and 28.22 min. along with the appearance of additional peaks most noticeably a peak at 29.52 minutes; therefore, the concentration of the hydroxylamine was left at 20 mg/mL.

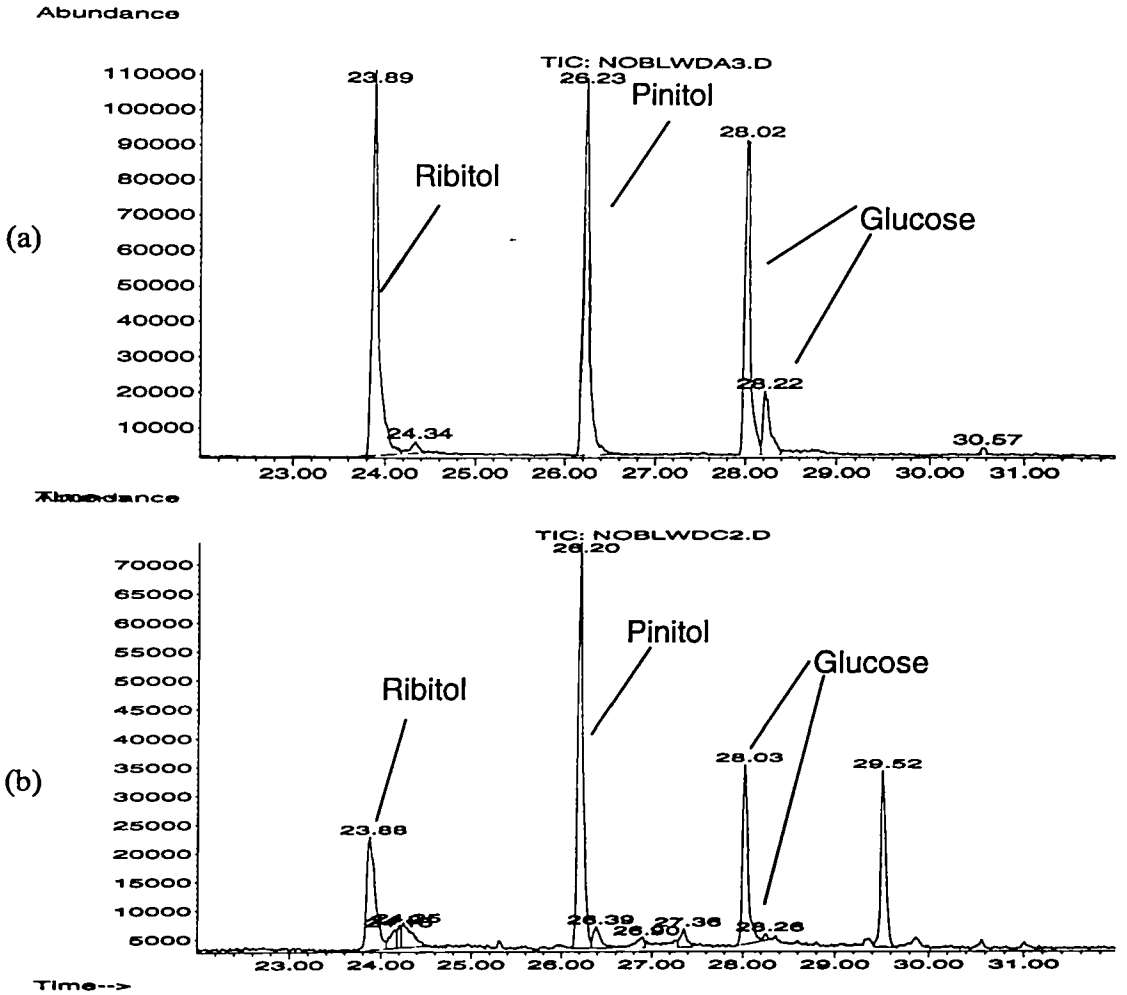


Figure 3-7. Comparison of the chromatograms produced from derivatizing glucose with $MeONH_2$•HCl/pyridine followed by MSTFA and $MeONH_2$•HCl/pyridine at concentrations of (a) 20 mg/mL and (b) 2 mg/mL .

3.1.5 Evaluation of the Volume of MSTFA Used

From examination of the peaks in Figure 3-7 the ratios of the different standards were not consistent, possibly indicating that the MSTFA reaction may not be going to completion. To test the reproducibility of the reaction three 5 μL aliquots of a MeOH

extract of an outdoor urban restaurant sample were derivatized using 5 μL of $MeONH_2$•HCl/pyridine followed by 5 μL of MSTFA as described above; three deuterated PAH internal standards were also added to the sample: acenapthalene-d_{10}, pyrene-d_{10}, and perylene-d_{12}. The peak areas of the major components were compared to the peak areas of these standards. If the MSTFA reaction was working reproducibly, the peak area ratios should remain constant in each sample. The ratios of the various compounds were found to vary significantly from run to run (Table 3-1), indicating that there may be not enough MSTFA to allow the reaction to go to completion.

This reaction was repeated with fresh window film extract samples (5 μL) using different volumes of MSTFA (5 μL, 10 μL, 15 μL, and 20 μL), preceded by a volume of $MeONH_2$•HCl/pyridine equal to that of MSTFA used. The results of these experiments are shown in Table 3-2. When using 10, 15 or 20 μL the ratios were quite similar, but consistently greater than the data from the 5 μL reactions. Another series of derivatizations was performed in triplicate using 20 μL volumes of the derivatizing solutions; these data are reported in Table 3-3. The low RSD's prompted us to standardize on 20 μL volumes for all derivatizations of window film extracts.

Table 3-1. Reproducibility of peak areas when using 5 µL of MSTFA and 5 µL of $MeONH_2$•HCl/pyridine.

	1	2	3				
Compound[e]	RATIO[a]	RATIO[a]	RATIO[a]		AVG[b]	STDEV[c]	RSD[d]
Arabinose 1	0.03	0.11	0.03		0.05	0.05	85%
Arabinose 2	0.11	0.29	0.10		0.17	0.11	64%
Xylitol	0.05	0.05	0.08		0.06	0.02	26%
Acenapthene-d_{10}	0.74	0.86	0.43		0.68	0.23	33%
Levoglucosan	0.19	0.42	0.30		0.30	0.12	39%
Pinitol	0.06	0.16	0.03		0.08	0.07	83%
L-Quebrachitol	0.09	0.14	0.08		0.11	0.03	29%
Fructose 1	0.98	1.95	1.21		1.38	0.51	37%
Fructose 2	0.47	1.19	0.60		0.75	0.38	50%
Glucose 1	0.31	1.04	0.40		0.58	0.40	69%
Glucose 2	0.06	0.32	0.06		0.15	0.15	100%
Myo-Inositol	0.04	0.40	0.04		0.16	0.21	130%
Pyrene-d_{10}	1.00	1.00	1.00		1.00	-	-
Sucrose	0.24	1.52	0.24		0.67	0.74	110%
Trehalose	0.03	0.13	0.01		0.05	0.06	120%
Perylene-d_{12}	0.38	0.40	0.47		0.42	0.05	12%

a: Ratio of compound peak area to peak area of pyrene-d_{10}.
b: AVG = average ratio from runs 1, 2 and 3.
c: STDEV = standard deviation.
d: RSD = relative standard deviation.
e: Compounds are in their oxime and/or TMS derivative forms.

Table 3-2. Reproducibility of peak areas using 5 μL, 10 μL, 15 μL and 20 μL of MSTFA with an equivalent amount of $MeONH_2$•HCl/pyridine.

	5 μL	10 μL	15 μL	20 μL				
Compound[e]	RATIO[a]	RATIO[a]	RATIO[a]	RATIO[a]		AVG[b]	STDEV[c]	RSD[d]
Arabinose 1	0.05	0.16	0.16	0.17		0.17	0.00	3%
Arabinose 2	0.09	0.78	0.46	0.61		0.62	0.16	26%
Xylitol	0.03	0.27	0.27	0.33		0.29	0.04	12%
Acenapthene-d_{10}	0.74	0.75	0.76	0.72		0.74	0.02	3%
Levoglucosan	0.09	0.39	0.45	0.62		0.48	0.12	24%
Pinitol	0.09	0.15	0.15	0.18		0.16	0.02	12%
L-Quebrachitol	0.08	0.12	0.12	0.13		0.12	0.01	6%
Fructose 1	1.38	2.92	3.12	3.24		3.09	0.16	5%
Fructose 2	1.03	1.57	2.20	2.19		1.99	0.36	18%
Glucose 1	1.05	1.27	1.81	1.65		1.58	0.28	18%
Glucose 2	0.27	0.40	0.50	0.54		0.48	0.07	15%
Myo-inositol	0.30	0.26	0.35	0.43		0.35	0.08	23%
Pyrene-d_{10}	1.00	1.00	1.00	1.00		1.00	-	-
Sucrose	1.39	1.61	2.05	2.32		1.99	0.35	18%
Trehalose	0.16	0.21	0.24	0.21		0.22	0.02	8%
Perylene-d_{12}	0.63	0.52	0.57	0.59		0.56	0.03	6%

a: Ratio of compound peak area to peak area of pyrene-d_{10}.
b: AVG = average ratio of peak areas using 10, 15 and 20 μL of MSTFA.
c: STDEV = standard deviation using 10, 15 and 20 μL of MSTFA .
d: RSD = relative standard deviation using 10, 15 and 20 μL of MSTFA.
e: Compounds are in their oxime and/or TMS derivative forms.

Table 3-3. Reproducibility of peak areas using 20 µL of MSTFA and 20 µL of $MeONH_2$•HCl/pyridine.

	20 µL	20 µL	20 µL				
Compound[e]	RATIO[a]	RATIO[a]	RATIO[a]		AVG[b]	STDEV[c]	RSD[d]
Arabinose 1	0.17	0.18	0.19		0.18	0.01	5%
Arabinose 2	0.61	0.67	0.65		0.65	0.03	5%
Xylitol	0.33	0.34	0.28		0.32	0.03	10%
Acenapthene-d_{10}	0.72	0.84	0.83		0.79	0.07	8%
Levoglucosan	0.62	0.70	0.65		0.66	0.04	6%
Pinitol	0.18	0.18	0.16		0.18	0.01	6%
L-Quebrachitol	0.13	0.14	0.14		0.14	0.01	5%
Fructose 1	3.24	4.02	3.67		3.64	0.39	11%
Fructose 2	2.19	2.62	2.43		2.41	0.21	9%
Glucose 1	1.65	2.22	1.86		1.91	0.29	15%
Glucose 2	0.54	0.57	0.53		0.55	0.02	4%
Myo-Inositol	0.43	0.45	0.44		0.44	0.01	3%
Pyrene-d_{10}	1.00	1.00	1.00		1.00	-	-
Sucrose	2.32	2.24	2.26		2.27	0.04	2%
Trehalose	0.21	0.16	0.17		0.18	0.03	14%
Perylene-d_{12}	0.59	0.58	0.57		0.58	0.01	2%

a: Ratio of compound peak area to peak area of pyrene-d_{10}.
b: AVG = average ratio of peak areas using 20 µL of MSTFA.
c: STDEV = standard deviation.
d: RSD = relative standard deviation.
e: Compounds are in their oxime and/or TMS derivative forms.

3.2 Addition of 9-Anthracenemethanol

9-Anthracenemethanol was introduced into all reaction mixtures to determine the extent of derivatization of alcohols by MSTFA. Both the alcohol and its TMS derivative are easily separated and detected under the analysis protocol. Should there be a problem with the trimethylsilylation reaction (Figure 3-8) the underivatized form of 9-anthracenemethanol would be observed in the chromatogram. The TMS derivative of 9-anthracenemethanol has a different retention time and mass spectrum than its underivatized form (Figure 3-9).

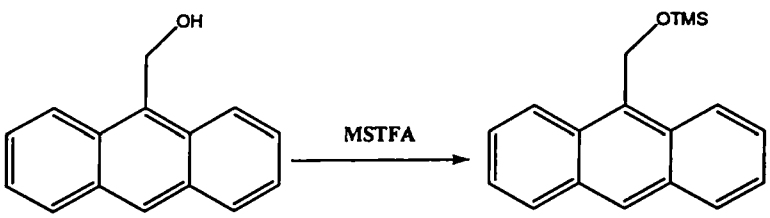


Figure 3-8. 9-Anthracenemethanol is readily converted to it trimethylsilyl derivative.

3.3 Silanization of GC Vials

One of the main disadvantages of trimethylsilylation as a derivatization method is that the TMS derivatives can be quite susceptible to hydrolysis. In the case of trace analyses performed on small scales, the potential for hydrolysis by trace amounts of water is rather high. Even traces of water in the GC vials themselves can result in some

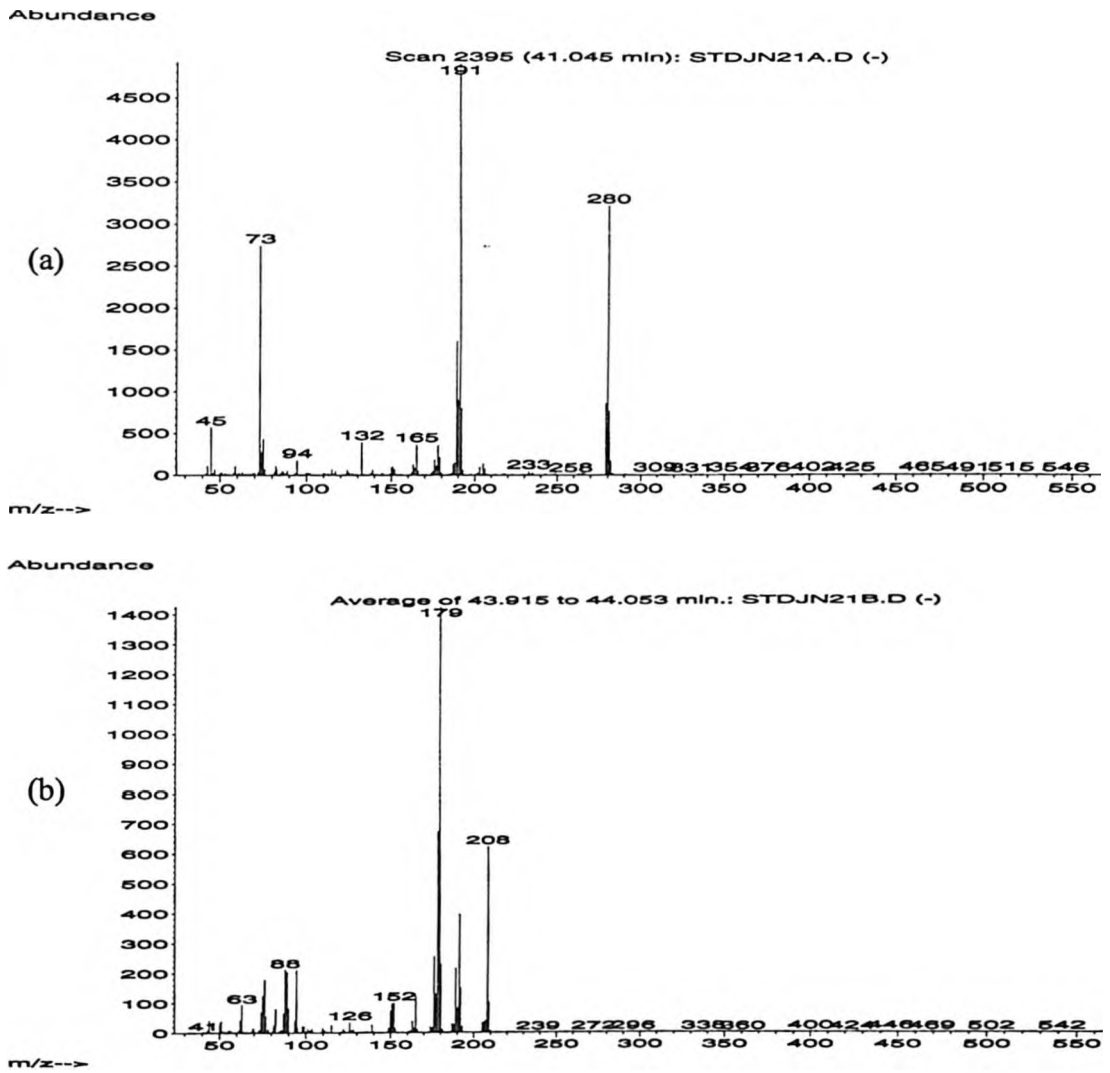


Figure 3-9. Mass spectra of (a) the trimethylsilyl ether of 9-anthracenemethanol (b) underivatized 9-anthracenemethanol.

hydrolysis, leading to significant lack of reproducibility. In our lab one solution to this problem was developed by J. Jia; she silanized the GC vials by treating the vials with dimethyldichlorosilane, $(CH_3)_2SiCl_2$ followed by methanol; the vials were dried and stored in a dessicator until needed. This procedure converted the Si-OH groups on the

surface of the glass to chlorosilyl ethers which when reacted with methanol produced a neutral methyl siloxane. The dried vials had very small amounts of moisture absorbed to the glass walls and, once implemented, gave very reproducible results. Instead of going through this silanization procedure we decided it may be easier and equally effective to redissolve the blown down derivatized mixture in a solution containing 80% toluene and 20% MSTFA. The presence of the 20% MSTFA should react with any traces of moisture that may be present and ensure that trimethylsilylation reactions had gone to completion.

3.3.1 Cleaning of GC-vials

Another concern about the GC vials was that other polar compounds similar to those found in the window film may be present in the vials already. Since we are analyzing for polar compounds on the surface of glass windows it is reasonable that there may be some of these compounds coming from the glass of the vial. Three reaction blanks were run in three vials that were cleaned differently. The first vial was a regular GC vial that was not cleaned or silanized in any way. The second GC vial was rinsed with DCM followed by methanol, and then placed in an oven at 170°C for 1 hour. The third vial was a solvent –rinsed and a silanized vial provided by J. Jia. Figure 3-10 shows an expanded region of the chromatograms where the monosaccharide TMS derivatives elute. There was no evidence of any sugar or sugar alcohol derivatives in these blank samples. Additionally, there were hardly any differences between the three vials; therefore, we concluded that the use of regular GC vials without any cleaning was acceptable for these analyses.

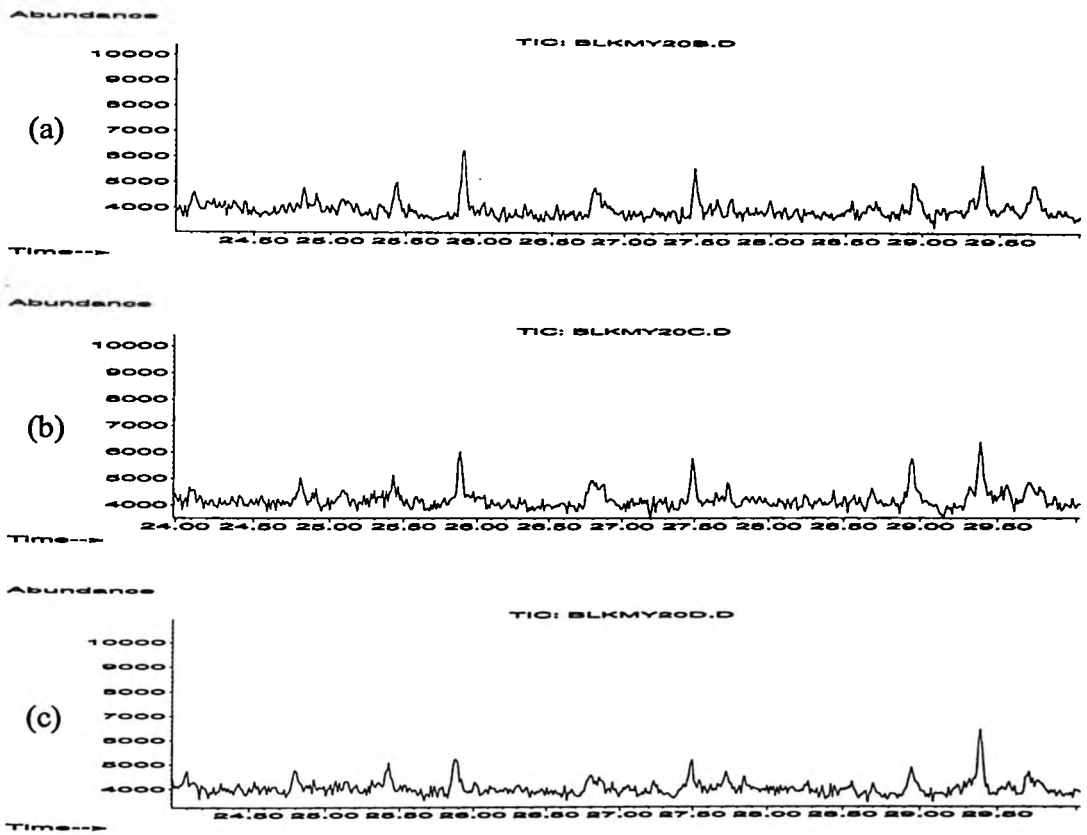


Figure 3-10. GC/MS chromatograms of reaction blanks performed using GC vials that had been cleaned differently: (a) no cleaning (b) rinsed with DCM and methanol then heated at 170°C for 1 hour (c) solvent-rinsed and silanized vial.

3.4 Determination of Relative Response Factors

Previously another member of our research group (J. Jia) had determined the relative response factors (RRF) for the derivatives of a number of metabolite standards. Some of the RRF values were redetermined as part of this study. The RRF values determined in this study and some of those determined by J. Jia are presented in Table 3-4. The values determined by J. Jia were typically lower than the ones determined in this

study. A number of reasons could account for these differences. First, her response factors were based only

Table 3-4. Comparison of relative response factors in TIC mode determined in this study versus a previous one.

Compound	AVG[a]	J. Jia[b]
Arabinose MeOX1-$(TMS)_4$	2.08	2.12
Arabinose MeOX2-$(TMS)_5$		
Xylitol-$(TMS)_5$	2.63	1.57
Acenapthene-d_{10}	1.01	n/a
Levoglucosan-$(TMS)_3$	1.55	n/a
Pinitol-$(TMS)_5$	2.13	1.72
L-Quebrachitol-$(TMS)_5$	2.29	1.30
Fructose MeOX1-$(TMS)_5$	2.34	1.15
Fructose MeOX2-$(TMS)_6$		
Glucose MeOX1-$(TMS)_5$	3.35	2.57
Glucose MeOX2-$(TMS)_6$		
Myo-Inositol-$(TMS)_6$	3.52	1.58
Pyrene-d_{10}	1.00	n/a
Sucrose-$(TMS)_8$	2.34	1.41
Trehalose-$(TMS)_8$	3.82	1.47
Maltitol-$(TMS)_9$	2.62	n/a
Perylene-d_{12}	0.79	n/a

a: AVG = average relative response factors determined in this study based on three experiments.
b: J. Jia = relative response factors determined previously by J. Jia based on a single experiment.

on single determinations. Second, the procedure used to derivatize the standards was slightly different. In J. Jia's procedure the standards were derivatized in a Reactivial (1 mL) and then an aliquot of the derivatized mixture was diluted into a separate GC vial. In this study all derivatizations and dilutions were done directly in a single GC vial. Third, the excess of MSTFA used was much greater in this study than in Jia's. In J. Jia's work

she had about an 8-fold excess of MSTFA, while in this study there was a much larger excess (>16,000 fold). Finally, since the RRF values were calculated in TIC mode some of the peak areas could be incorrect due to interferences. All of these factors could result in greater responses and thus larger response factors in this study. Calculating response factors using mass chromatograms is much more reliable and these values were used rather than the TIC peak areas. Unfortunately, J. Jia did not determine response factors using mass chromatograms so direct comparisons could not be made.

3.5 Retention Index Standards

A series of odd-carbon number fatty acids were added to each sample. The derivatization procedure converted these compounds to their trimethylsilyl esters. These TMS esters were used as retention index markers for retention index determination. The retention time differences between neighbouring pairs of these fatty acid esters were very consistent (Table 3-5). Due to the "dirty" nature of the window film samples, peaks corresponding to the fatty acid ester retention index standards were sometimes obscured by peaks in the sample matrix. Often the fatty acid TMS esters eluting after C_{15} were not observed in the chromatogram. When this situation occurred the retention time of the missing fatty acid TMS ester was estimated by using one of the values found in Table 3-5.

Table 3-5. Differences between fatty acid TMS esters

	1	2	3	4				
Fatty Acid TMS Esters	Difference	Difference	Difference	Difference		AVG[a]	STDEV[b]	RSD[c]
C_7-C_9	4.84	4.86	4.75	4.67		4.78	0.0876	1.83%
C_9-C_{11}	4.53	4.55	4.52	4.50		4.53	0.0208	0.46%
C_{11}-C_{13}	4.17	4.22	4.14	4.17		4.18	0.0332	0.79%
C_{13}-C_{15}	3.81	3.88	3.81	3.79		3.82	0.0395	1.03%
C_{15}-C_{19}	6.77	6.88	6.74	6.78		6.79	0.0608	0.89%
C_{19}-C_{23}	5.83	5.95	5.81	5.82		5.85	0.0655	1.12%
C_{23}-C_{27}	5.09	5.22	5.08	5.07		5.12	0.0705	1.38%
C_{27}-C_{31}	4.48	4.62	4.52	4.48		4.53	0.0661	1.46%

a: AVG = average difference between fatty acid TMS esters using runs 1, 2, 3 and 4.
b: STDEV = standard deviation
c: RSD = relative standard deviation

3.6 Summary of Analytical Method for Window Film Samples

Detailed procedures for the derivatization of the window films samples can be found in the experimental section (Section 2.7.1 and Section 2.7.2). The analytical method developed has been found to be reproducible on a small scale. Several procedures in the method will help ensure that the derivatization reactions go to completion: (1) addition of 9-anthracenemethanol and (2) use of toluene/MSTFA (80:20) solution as the "solvent" to take up silylated residues after blowing down reaction mixtures.

4.0 RESULTS AND DISCUSSION

In this chapter the results of the analysis of polar compounds identified in samples collected from untinted windows in the Toronto area will be discussed. The samples analyzed were collected in March 2001 at sites along an urban-rural gradient (Figure 4-1), from both indoor and outdoor windows. Sampling sites included offices, a residence, a laboratory and a restaurant. The major issues which will be presented in this chapter include: (1) the criteria used to establish a positive identification of a compound, (2) the possible sources of the identified compounds, (3) the contribution of the polar compounds to the overall mass of the organic films and (4) the reproducibility of the results.

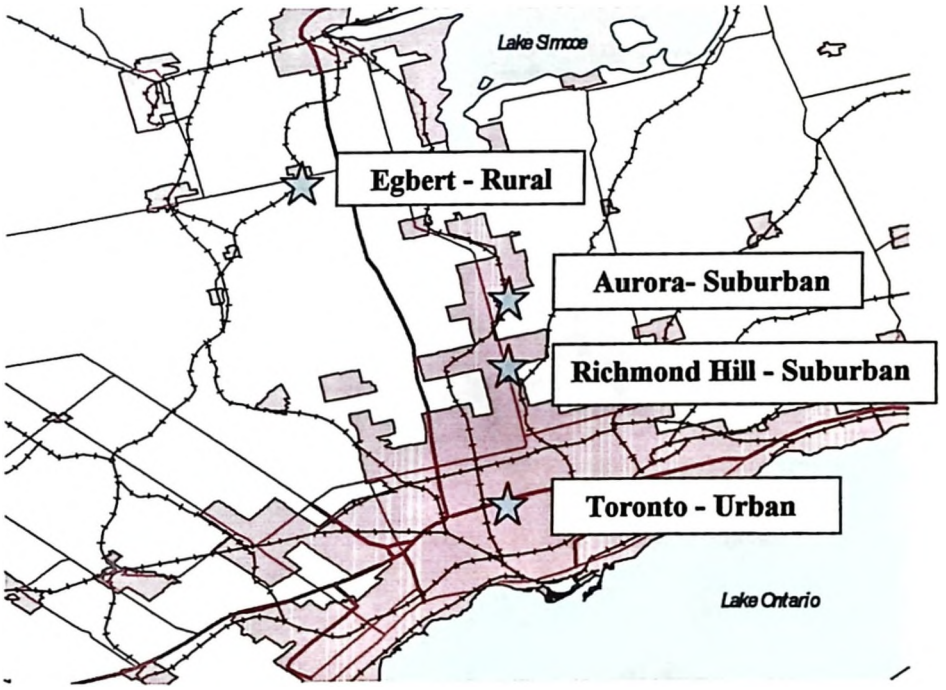


Figure 4-1. Map showing the urban-rural gradient along which the samples were collected.

Figures 4-2a and 4-2b represent portions of the total ion chromatograms for a typical derivatized window film sample after methoximation followed by trimethylsilylation. This chromatogram shows that fructose, glucose and sucrose (all off-scale) are the major compounds in this mixture. A number of minor components were also identified. The chromatographic quality of this analysis is typical of all analyses. However, these samples were sufficiently "dirty" that chromatographic performance deteriorated rather quickly necessitating routine cutting of the retention gap to ensure that good chromatographic performance was maintained from run to run.

4.1 Criteria for Identification of Compounds

One of the main foci of this work was to be able to identify as many of the peaks in the GC/MS chromatograms as possible. Criteria were established in order to classify peaks as (1) positively identified, (2) tentatively identified or (3) unknown. A positive identification of a compound was made when there was a retention index match and a mass spectral match to a derivatized authentic standard; in many cases, there was also a good mass spectral match to a mass spectrum in a commercial mass spectral library (Wiley and/or NIST 2002). The retention index of the peak had to fall within two standard deviations ($\pm 2\sigma$) of the mean retention index value from analyses of authentic standards. Due to the "dirty" nature of the film samples (which had no cleanup prior to derivatization and analysis), the sample matrix sometimes caused increases in peak widths, retention times and retention index values. Therefore, in some cases positive

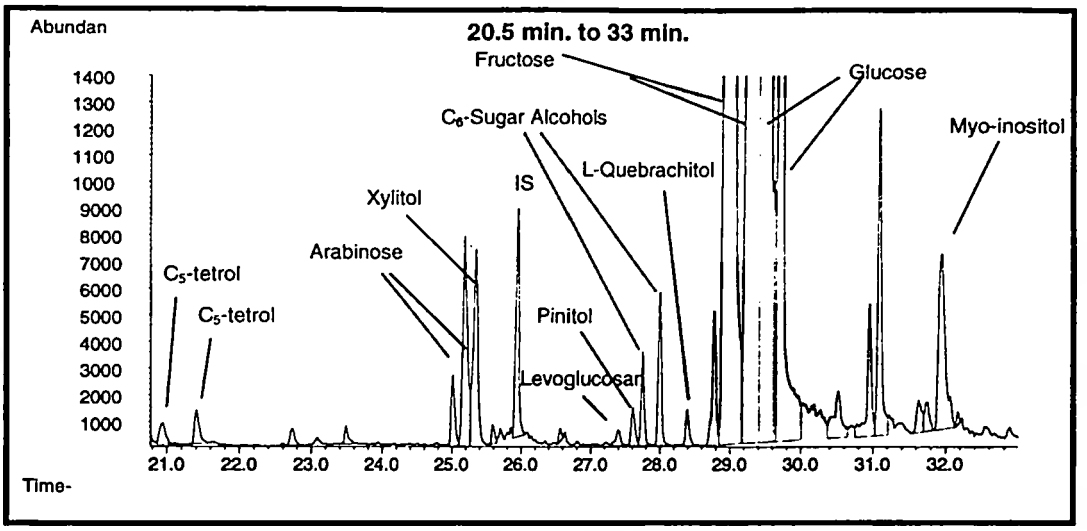


Figure 4-2a. Typical total ion chromatogram of compounds identified within the range of 20.5 min. to 33 min. in window film samples.

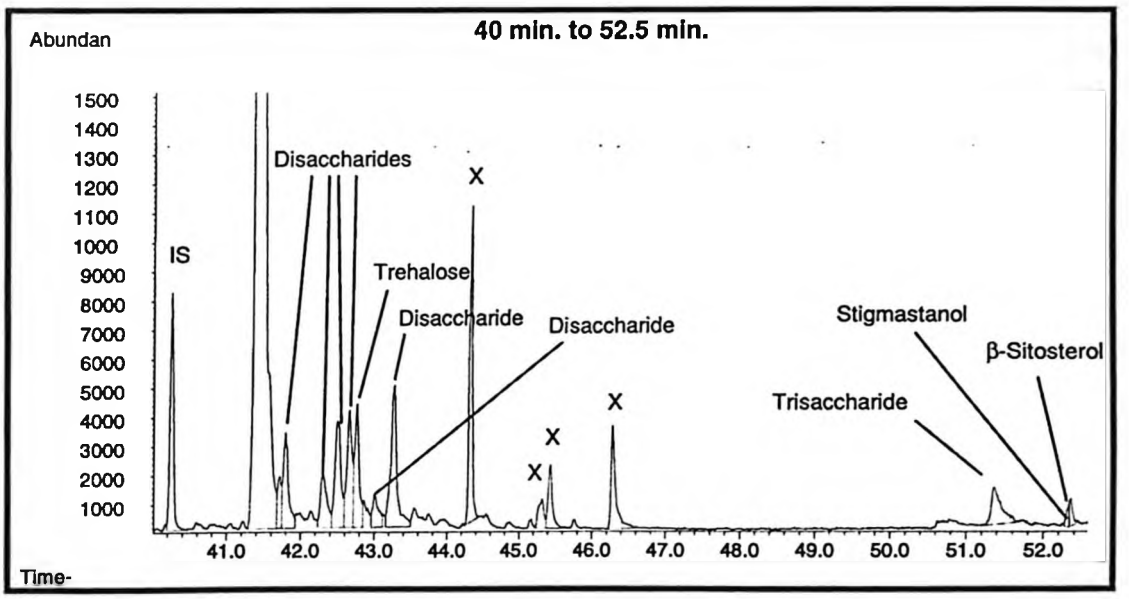


Figure 4-2b. Typical total ion chromatogram of compounds identified within the time range of 40 min. to 52.5 min. in window film samples. (x = peaks resulting from the reaction blank and IS = internal standard)

identifications were still made even though the retention index value was somewhat outside the 2σ range. In all cases of a positive identification the mass spectral match had to be very good (>95%). A tentative identification was made when an authentic standard was unavailable but there was a good mass spectral match (>80%) to a spectrum in a commercial mass spectral library (Wiley and/or NIST 2002). In some cases a compound class could be identified (e.g., a hexose) but the specific isomer was not available as an authentic standard. Unknowns were all peaks which did not meet the above criteria.

4.2 Reproducibility of Retention Index Values

4.2.1 Reproducibility in Window Film Extracts

The reproducibilities of retention index values were determined by comparing the values obtained from three separate analyses of a derivatized methanol extract of a window film sample. However, since some samples were available in rather limited amounts, repeat analyses were not performed on these samples. The methanol extract of an outdoor urban restaurant window film (JRO) was analyzed the most frequently because it was the most abundant sample. It was assumed that if the retention index values of the outdoor restaurant sample were reproducible then the other film samples would likely give results that were just as reproducible. Table 4-1 shows the retention index values determined on the JRO samples on three different dates: October 8/03, March 15/04 and September 27/04. The results show that the values are quite reproducible with relative standards deviations less than 0.55%.

Table 4-1. Retention index values of compounds identified in an outdoor urban restaurant sample (JRO) from analyses performed on Oct. 8/03, Mar. 15/04, and Sept. 27/04. The averages (AVG), standard deviations (STDEV) and relative standard deviations (RSD) were calculated.

Compounds (as $MeONH_2$/TMS Derivatives)	October 8/03	March 15/04	September 27/04		AVG	STDEV	RSD
glycerol	768.2	766.7	771.9		769.0	2.7	0.4%
C_5-tetrol	996.6	1004.9	995.2		998.9	5.2	0.5%
C_5-tetrol	1016.9	1025.3	1014.9		1019.0	5.6	0.6%
Arabinose 1	1189.4	1194.5	1190.01		1191.3	2.8	0.2%
Arabinose 2	1197.1	1202.2	1197.8		1199.0	2.7	0.2%
Xylitol	1204.8	1212.8	1205.6		1207.7	4.4	0.4%
Levoglucosan	1306.3	1310.5	1307.9		1308.2	2.1	0.2%
Pinitol	1315.7	1323.0	1316.8		1318.5	3.9	0.3%
L-Quebrachitol	1357.1	1363.4	1357.9		1359.4	3.4	0.3%
Fructose 1	1384.3	1391.1	1386.8		1387.4	3.4	0.3%
Fructose 2	1400.0	1406.8	1403.7		1403.3	3.4	0.2%
Glucose 1	1409.4	1416.2	1413.7		1413.1	3.4	0.2%
Glucose 2	1421.5	1427.2	1423.7		1424.1	2.9	0.2%
Myo-inositol	1546.8	1557.1	1548.9		1551.0	5.5	0.4%
Sucrose	2139.3	2144.1	2138.0		2140.5	3.2	0.2%
Trehalose	2233.8	2235.7	2229.6		2233.0	3.1	0.1%
Stigmastanol	3004.6	3008.2	3002.9		3005.2	2.7	0.1%

4.3 Comparison of Retention Index Values from Window Film Samples and Authentic Standards

The retention index values and the standard deviations of over 100 authentic derivatized metabolite standards were determined previously by J. Jia[9]. Retention index values for the plant sterols stigmastanol, β-sitosterol and the C_5-tetrols were determined in this study. Using these values, 21 different compounds were identified positively in the methanol extracts of the window films. Tables 4-2 show that the majority of

identified peaks typically fall within $\pm 2\sigma$ of the retention index value of the corresponding derivatized authentic standard. The highlighted values indicate retention indices that are greater than $\pm 3\sigma$. One factor that could contribute to this is the sample matrix. The "dirty" nature of the samples often led to rapid degradation of the chromatographic performance of the column. In addition, some peaks were heavily overloaded which would increase the retention times and thus the retention indeces.

4.4 Positively Identified Compounds and Their Possible Sources

The total numbers of peaks identified in any film sample varied from 25 to 49 peaks. In the outdoor window film samples the peaks which were positively identified constituted 75-90% of the peak area in the total ion chromatogram. The indoor window film samples positively identified peaks which corresponded to about 75-79% of the total peak area. The number of tentatively identified peaks ranged from 2 to 9 peaks while the number of unknowns ranged from 5 to 20 peaks. A summary of these results can be found in Table 4-3. Appendix 2 lists the retention index values for positive, tentative and unknown compounds found in all of the window film samples analyzed.

Table 4-2. Retention index values of identified compounds found in window films at outdoor sites (EBO, DWO, PHWO, SRO RSO, JRO) and at indoor sites (EBI, DWI, PHWI, SRI, RSI, JRI) compared to authentic standards (RI). Highlighted values have a difference greater than three standard deviations (3σ)

Identified Compound	RI of Standards[a]	STDEV (σ)[a]	Rural Office (EBO)	# of σ's from RI of Standard	Suburban Office (DWO)	# of σ's from RI of Standard	Urban Laboratory (PHWO)	# of σ's from RI of Standard
glycerol	768.6	1.6						
benzoic acid	864.3	1.2						
glyceric acid	871.7	1.4						
fumaric acid	888.1	0.6						
succinic acid	904.1	0.4						
C_5-tetrol[b]	997.1	0.4	999.8	7.4	1000.9	10.5	1002.4	14.8
C_5-tetrol[b]	1016.7	0.4	1019.1	6.7	1020.1	9.4	1021.1	12.1
malic acid	1058.5	0.9						
adipic acid	1106.7	n/a						
Arabinose 1	1194.7	1.5	1192.8	-1.3	1191.8	-1.9	1194.0	-0.5
Arabinose 2	1202.4	1.5	1200.5	-1.3	1200.5	-1.3	1201.7	-0.5
Xylitol	1204.5	4.7	1209.7	1.1	1208.2	0.8	1213.3	1.9
Levoglucosan	1307.3	n/a	1307.9		1307.9		1308.4	
Pinitol	1315.7	1.9	1319.9	2.2	1318.8	1.7	1321.5	3.0
L-Quebrachitol	1356.9	2.6	1359.8	1.1	1359.7	1.1	1361.8	1.9
Fructose 1	1394.0	3.4	1389.2	-1.4	1390.1	-1.2	1388.5	-1.6
Fructose 2	1406.1	3.5	1405.0	-0.3	1404.7	-0.4	1403.7	-0.7
Glucose 1	1409.7	2.4	1416.5	2.8	1418.3	3.6	1413.6	1.6
Glucose 2	1421.3	2.4	1426.0	2.0	1427.7	2.7	1425.1	1.6
Myo-Inositol	1552.5	5.0	1549.5	-0.6	1550.7	-0.4	1553.6	0.2
Sucrose	2139.2	6.3	2139.3	0.0	2140.0	0.1	2137.3	-0.3
Trehalose	2231.6	2.8	2231.6	0.0	2230.3	-0.5	2233.7	0.7
Stigmastanol[b]	3007.9	2.3	3002.9	-2.2				
β-Sitosterol[b]	3012.2	2.1						

a. Retention Index (RI) and Standard Deviations (σ) for standards determined by J. Jia[9]

b. Retention Index (RI) and Standard Deviations (σ) determined in this study.

Table 4-2 (continued)

Identified Compound	RI of Standards[a]	STDEV (σ)[a]	Urban Office (SRO)	# of σ's from RI of Standard	Urban Residence (RSO)	# of σ's from RI of Standard	Urban Restaurant (JRO)[c]	# of σ's from RI of Standard
glycerol	768.6	1.6	765.3	-2.1	766.9	-1.0	769.0	0.2
benzoic acid	864.3	1.2						
glyceric acid	871.7	1.4						
fumaric acid	888.1	0.6						
succinic acid	904.1	0.4						
C_5-tetrol[b]	997.1	0.4	997.3	0.6	998.0	2.5	998.9	5.0
C_5-tetrol[b]	1016.7	0.4	1017.3	1.7	1017.3	1.7	1019.0	6.4
malic acid	1058.5	0.9						
adipic acid	1106.7	n/a						
Arabinose 1	1194.7	1.5	1189.4	-3.5	1190.8	-2.6	1191.3	-2.3
Arabinose 2	1202.4	1.5	1198.1	-2.9	1199.0	-2.2	1199.0	-2.2
Xylitol	1204.5	4.7	1205.8	0.3	1206.8	0.5	1207.7	0.7
Levoglucosan	1307.3	n/a	1306.3		1307.9		1308.2	
Pinitol	1315.7	1.9	1315.7	0.0	1317.9	1.2	1318.5	1.5
L-Quebrachitol	1356.9	2.6	1355.6	-0.5	1358.9	0.8	1359.4	1.0
Fructose 1	1394.0	3.4	1388.7	-1.6	1386.3	-2.3	1387.4	-1.9
Fructose 2	1406.1	3.5	1403.9	-0.6	1402.6	-1.0	1403.3	-0.8
Glucose 1	1409.7	2.4	1418.6	3.7	1413.2	1.4	1413.1	1.4
Glucose 2	1421.3	2.4	1427.0	2.4	1423.7	1.0	1424.1	1.2
Myo-Inositol	1552.5	5.0	1547.1	-1.1	1551.8	-0.1	1551.0	-0.3
Sucrose	2139.2	6.3	2137.9	-0.2	2137.3	-0.3	2140.5	0.2
Trehalose	2231.6	2.8	2228.2	-1.2	2231.6	0.0	2233.0	0.5
Stigmastanol[b]	3007.9	2.3	3001.1	-2.9	3005.5	-1.0	3005.2	-1.2
β-Sitosterol[b]	3012.2	2.1	3004.6	-3.7				

a. Retention Index (RI) and Standard Deviations (σ) for standards determined by J. Jia[9]
b. Retention Index (RI) and Standard Deviations (σ) determined in this study.
c. Retention Index (RI) values for JRO are an average of 3 experiments

Table 4-2 (continued)

Identified Compound	RI of Standards[a]	STDEV (σ)[a]	Rural Office (EBI)	# of σ's from RI of Standard	Suburban Office (DWI)	# of σ's from RI of Standard	Urban Laboratory (PHWI)	# of σ's from RI of Standard
glycerol	768.6	1.6	770.3	1.1	769.0	0.3		
benzoic acid	864.3	1.2	864.9	0.5				
glyceric acid	871.7	1.4	869.0	-1.9	869.0	-1.9		
fumaric acid	888.1	0.6	889.1	1.7				
succinic acid	904.1	0.4			902.2	-4.6	902.7	-3.6
C_5-tetrol[b]	997.1	0.4						
C_5-tetrol[b]	1016.7	0.4						
malic acid	1058.5	0.9	1057.5	-1.1				
adipic acid	1106.7	n/a	1107.7		1106.3			
Arabinose 1	1194.7	1.5	1192.5	-1.5	1193.7	-0.7	1193.5	-0.8
Arabinose 2	1202.4	1.5	1200.7	-1.1	1201.4	-0.6	1202.2	-0.2
Xylitol	1204.5	4.7	1210.4	1.2	1213.5	1.9	1209.9	1.1
Levoglucosan	1307.3	n/a	1308.9		1306.8		1307.3	
Pinitol	1315.7	1.9	1321.0	2.8	1323.6	4.2	1320.4	2.5
L-Quebrachitol	1356.9	2.6	1361.4	1.7	1363.5	2.5	1360.2	1.3
Fructose 1	1394.0	3.4	1389.8	-1.2	1390.3	-1.1	1386.9	-2.1
Fructose 2	1406.1	3.5	1405.5	-0.2	1405.5	-0.2	1402.6	-1.0
Glucose 1	1409.7	2.4	1414.4	2.0	1415.0	2.2	1413.1	1.4
Glucose 2	1421.3	2.4	1425.5	1.7	1427.0	2.4	1423.6	0.9
Myo-Inositol	1552.5	5.0	1550.7	-0.4	1554.2	0.3	1551.8	-0.1
Sucrose	2139.2	6.3	2145.6	1.0	2143.4	0.7	2139.6	0.1
Trehalose	2231.6	2.8	2236.9	1.9	2239.1	2.7	2228.3	-1.2
Stigmastanol[b]	3007.9	2.3						
β-Sitosterol[b]	3012.2	2.1						

a. Retention Index (RI) and Standard Deviations (σ) for standards determined by J. Jia[9]

b. Retention Index (RI) and Standard Deviations (σ) determined in this study.

Table 4-2 (continued)

Identified Compound	RI of Standards[a]	STDEV (σ)[a]	Urban Office (SRI)	# of σ's from RI of Standard	Urban Residence (RSI)	# of σ's from RI of Standard	Urban Restaurant (JRI)	# of σ's from RI of Standard
glycerol	768.6	1.6			771.1	1.6	766.1	-1.6
benzoic acid	864.3	1.2						
glyceric acid	871.7	1.4			865.7	-4.3		
fumaric acid	888.1	0.6						
succinic acid	904.1	0.4	902.7	-3.6	903.1	-2.5	902.2	-4.7
C_5-tetrol[b]	997.1	0.4						
C_5-tetrol[b]	1016.7	0.4						
malic acid	1058.5	0.9			1057.9	-0.7		
adipic acid	1106.7	n/a			1107.2			
Arabinose 1	1194.7	1.5			1192.0	-1.8		
Arabinose 2	1202.4	1.5			1200.2	-1.4		
Xylitol	1204.5	4.7			1209.9	1.1		
Levoglucosan	1307.3	n/a	1307.3		1307.9		1307.4	
Pinitol	1315.7	1.9			1318.4	1.4		
L-Quebrachitol	1356.9	2.6			1359.3	0.9	1361.6	1.8
Fructose 1	1394.0	3.4	1389.2	-1.4	1387.1	-2.0	1388.9	-1.5
Fructose 2	1406.1	3.5	1405.5	-0.2	1403.4	-0.8	1404.2	-0.5
Glucose 1	1409.7	2.4	1413.9	1.8	1413.9	1.8	1414.2	1.9
Glucose 2	1421.3	2.4	1426.0	2.0	1424.9	1.5	1425.8	1.9
Myo-Inositol	1552.5	5.0	1554.7	0.4	1551.0	-0.3	1551.6	-0.2
Sucrose	2139.2	6.3	2143.0	0.6	2139.7	0.1	2138.5	-0.1
Trehalose	2231.6	2.8	2231.1	-0.2	2230.7	-0.3	2229.7	-0.7
Stigmastanol[b]	3007.9	2.3						
β-Sitosterol[b]	3012.2	2.1						

a. Retention Index (RI) and Standard Deviations (σ) for standards determined by J. Jia[9]

b. Retention Index (RI) and Standard Deviations (σ) determined in this study.

4.4.1 Mass Spectral Fragmentation Patterns of Sugar Derivatives

Using the methoximation/silylation procedure followed by GC/MS analysis described previously, a number of sugars (monosaccharides and disaccharides) and sugar alcohols were positively identified. Typically the mass spectrum of a trimethylsilyl derivative shows an $[M-15]^+$ ion due to the facile loss of a methyl group from the molecular ion[14]. In the case of sugar derivatives neither the molecular ion nor the $[M-15]^+$ ion were observed. Ions at *m/z* 73 and 147 were commonly observed, but these ions are characteristic ions derived from a TMS group and do not provide information about the structure of the molecule[14,15]. Hexoses produced intense ions at m/z 205, 217, and 319 as well as a weaker ion at m/z 103. Pentoses were characterized by intense ions at *m/z* 103, 217, and 307. C_5 and C_6 sugar alcohol TMS derivatives had ions at *m/z* 205, 217, 307 and 319. Inositols had intense peaks at m/z 217, 308 and 319. Disaccharides were characterized by a peak at *m/z* 361. Using these mass spectral fragmentation patterns tentative identifications could be made. Figure 3a shows the mass chromatogram of the m/z 361 ion, which should show all of the disaccharide derivatives in the sample. Two of the peaks have been positively identified as sucrose and trehalose. The other peaks in the mass chromatogram show mass spectral patterns similar to that of sucrose (Figure 3b); for example Figure 3c shows the mass spectrum of the peak at 43.27 min., which is similar to sucrose. This peak was therefore tentatively identified as being a disaccharide. Appendix 1 shows the derivatized structures of the positively identified compounds.

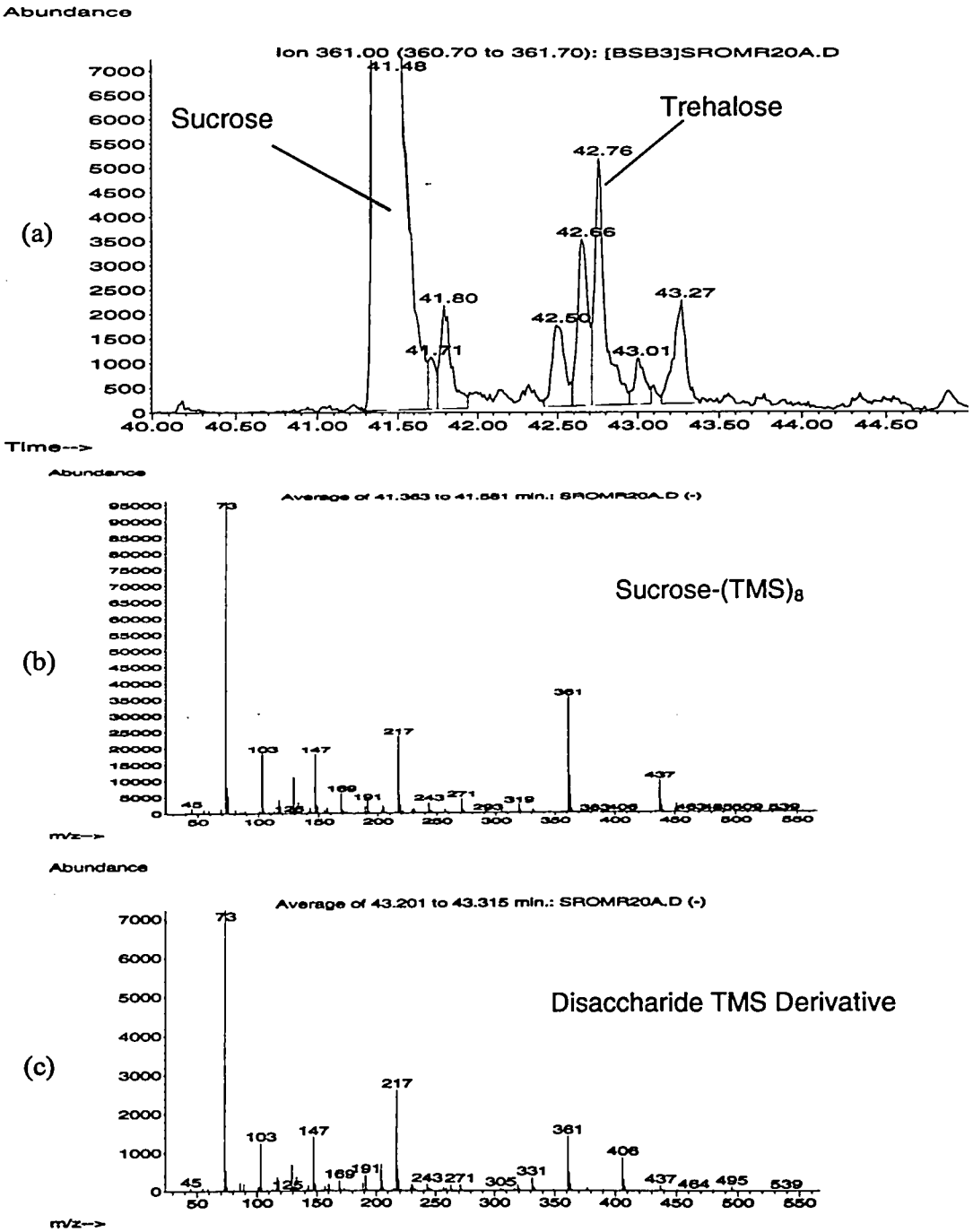


Figure 4-3. (a) Mass Chromatogram of m/z 361 ions. (b) Mass spectrum of sucrose. (c) Mass spectrum of a peak tentatively identified as a disaccharide.

Table 4-3. Summary of the positively identified tentatively identified and unknowns in indoor and outdoor window film samples at various sites.

	Positive Identifications		Tentative Identifications		Unknowns		
Sample Name	# of Peaks	% of Total Peak Area	# of Peaks	% of Total Peak Area	# of Peaks	% of Total Peak Area	Total # of Peaks
INDOOR SAMPLES							
Indoor Rural Office (EBI)	23	75.0%	9	8.6%	18	16.4%	50
Indoor Suburban Office (DWI)	19	79.0%	3	4.7%	5	16.3%	27
Indoor Urban Laboratory (PHWI)	16	79.1%	8	10.7%	19	10.3%	43
Indoor Urban Office (SRI)	13	76.5%	2	1.9%	14	21.6%	29
Indoor Urban Residence (RSI)	22	78.8%	8	10.9%	11	10.4%	41
Indoor Urban Restaurant (JRI)	14	78.2%	2	5.3%	8	16.5%	24
OUTDOOR SAMPLES							
Outdoor Rural Office (EBO)	16	90.8%	5	3.5%	6	5.7%	27
Outdoor Suburban Office (DWO)	16	88.9%	9	4.8%	8	6.3%	33
Outdoor Urban Laboratory (PHWO)	15	86.7%	4	2.4%	4	10.9%	23
Outdoor Urban Office (SRO)	18	88.6%	9	3.5%	11	7.9%	38
Outdoor Urban Residence (RSO)	17	80.5%	3	3.1%	10	16.4%	30
Outdoor Urban Restaurant #1 (JRO)	17	80.1%	8	6.3%	10	13.6%	35
Outdoor Urban Restaurant #2 (JRO)	17	79.7%	6	5.9%	11	14.4%	34
Outdoor Urban Restaurant #3 (JRO)	19	74.9%	5	5.1%	11	20.0%	35
Total Number of Unique Peaks							103

4.4.2 Sources of Compounds Identified in Film Samples

4.4.2.1 Possible Sources of Sugars and Sugar Alcohols

Previous work by our group showed that the PAH distribution in the window films resembles that of "aged" urban air[40]. Recently, Simoneit et al. reported the presence of sugars in aerosol samples taken in Sapporo, Japan at urban, rural and marine locales[19]. Saccharides have also been reported to be present in aerosols at other locations including Santiago, Chile[20], Kuala Lumpur, Malaysia[21], Ghent, Belgium[7], Rondonia, Brazil[23, 24], and Datong, China[21]. Many of the sugars reported by Simoneit et al. are identical to those observed in the window films of this study: levoglucosan, glucose, fructose, xylitol, glycerol, inositols, sucrose and trehalose (mycose)[19]. Simoneit claims the sources of these compounds to be from soils and their associated microbiota. Plant detritus is considered to be a major source of the organic matter in soil[41].

In aerosol samples the dominant saccharides observed were glucose, sucrose and trehalose (mycose)[19], whereas in the window films glucose, fructose and sucrose dominate. Another possible source that may be contributing to the levels of saccharides is plant nectar. Plant nectars have been shown to contain high levels of glucose, fructose and sucrose, similar to what is observed in the window films[25,26,27]. The confirmation of plants as a major (if not exclusive) source of the film material was the identification of these plant-derived sterols, stigmastanol and β-sitosterol, in the film samples. Another common plant sterol, stigmasterol, was not detected in the window film samples. Trehalose and some sugar alcohols have been proposed as products of fungal metabolism[28]. The presence of ergosterol, a sterol unique to fungi, would confirm the

presence of fungal-derived components in the window film[29]. However, no ergosterol was detected in any of the samples analyzed so it is unlikely that fungal metabolites contribute much if anything to the window films.

4.4.2.2 Source of Levoglucosan

Levoglucosan, a 1,6-anhydro derivative of glucose, is produced during the pyrolysis of cellulose[32] and has been used as a tracer for biomass burning[33-35] (Figure 4-4). Major ions in the mass spectrum of the TMS derivative of levoglucosan (*m/z* 378) are *m/z* 204, *m/z* 217 and *m/z* 333. The fragments are produced from the losses of $C_7H_{18}OSi_2$ (m/z 204), $C_6H_{17}OSi_2$ (m/z 217) and CH_3Si (*m/z* 333)[36]. Mannosan and galactosan are two other anhydrosugars produced during the pyrolysis of cellulose, however they were not detected in the film samples.

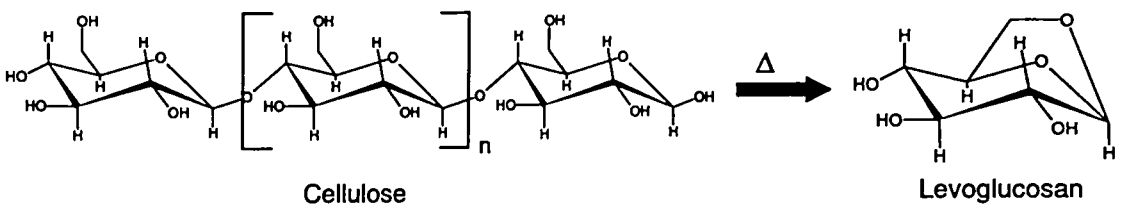


Figure 4-4. Production of levoglucosan from the pyrolysis of cellulose.

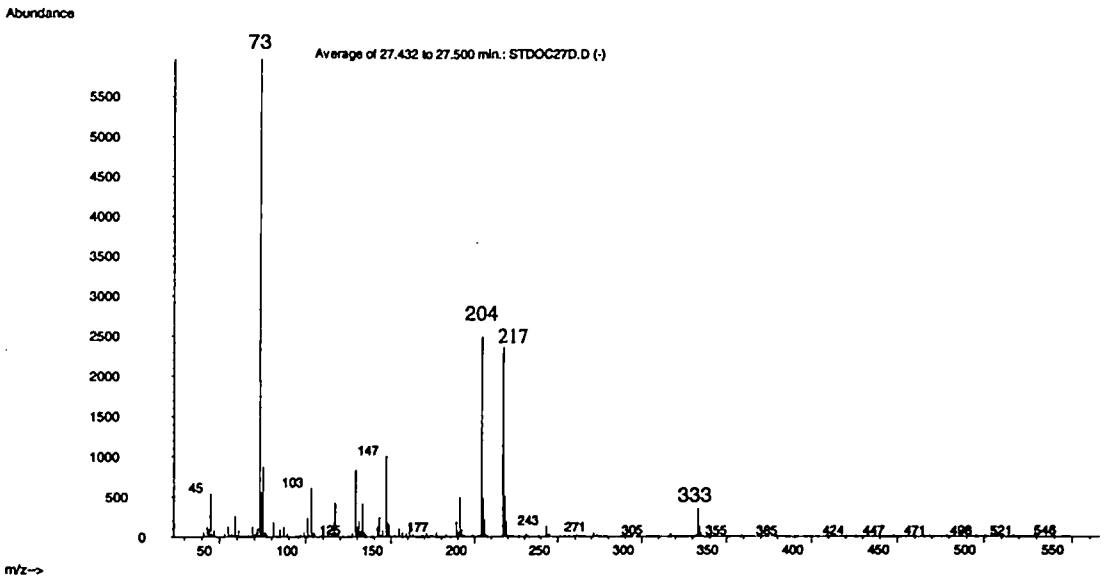


Figure 4-5. Mass spectrum of levoglucosan-(TMS)$_3$.

4.4.2.3 Source of the C_5-tetrols

Claeys et al. recently described a new pathway for the formation of two major constituents of secondary organic aerosols through the complex photooxidation of isoprene[37]. Isoprene represents almost 50% of all biogenic non-methane hydrocarbons on the global scale[39]. Hydroxyl-radical initiated photooxidation of isoprene leads to the formation of two diastereometric tetrols: 2-methylthreitol and 2-methylerythritol (Figure 4-6).

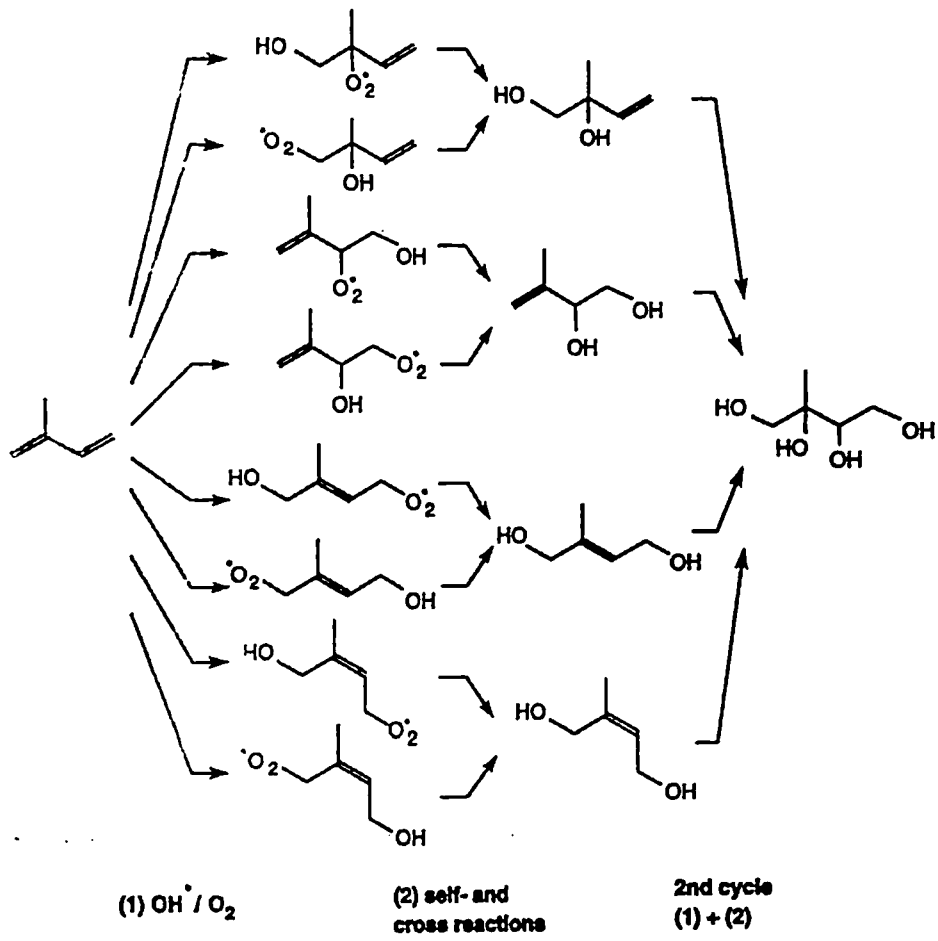


Figure 4-6. Proposed reaction of isoprene in the atmosphere to yield 2-methyltetrols by Claeys et al.[37].

Due to the large amounts of isoprene in the atmosphere we predicted that the 2-methyltetrols would probably be present in the window films. The possible presence of 2-methylthreitol and 2-methylerythritol was implicated by two chromatographic peaks at 20.06 and 20.52 min., respectively; the mass spectra of these peaks were consistent with tetra-TMS derivatives of five-carbon tetrols (Figure 4-7). Their existence was confirmed

by synthesizing an authentic mixture of the two tetrols from 2-methylvinyloxirane (Section 2.9). The expected *m/z* of the C_5-tetrols was expected to be 136. The mass spectrum of the synthesized compounds using a GC-TOF showed a mass at *m/z* 105, which was most likely the loss of $^{\bullet}CH_2OH$. The elemental composition of m/z was determined to be $C_4H_9O_3$ within 16 ppm (Appendix 3). Spectra from the ^{1}H-NMR showed chemical shifts that corresponded well to the structure of the C_5-tetrols (Appendix 3). A drop of D_2O to the sample caused the hydroxyl group peaks (4-4.7 ppm) to disappear. The ^{13}C-NMR spectrum matched well to the theoretical chemicals shifts calculated using ACD labs NMR software (Appendix 3). The mass spectra of the TMS derivatives of the tetrols show key ions at *m/z* 219, *m/z* 117, and *m/z* 129. Figure 4-8 shows the fragmentation scheme for these TMS derivatives proposed by Claeys et al[38]. The tetrols were observed only in the outdoor window film samples (not in the indoor samples) and typically in a 2:1 ratio (Figure 4-7).

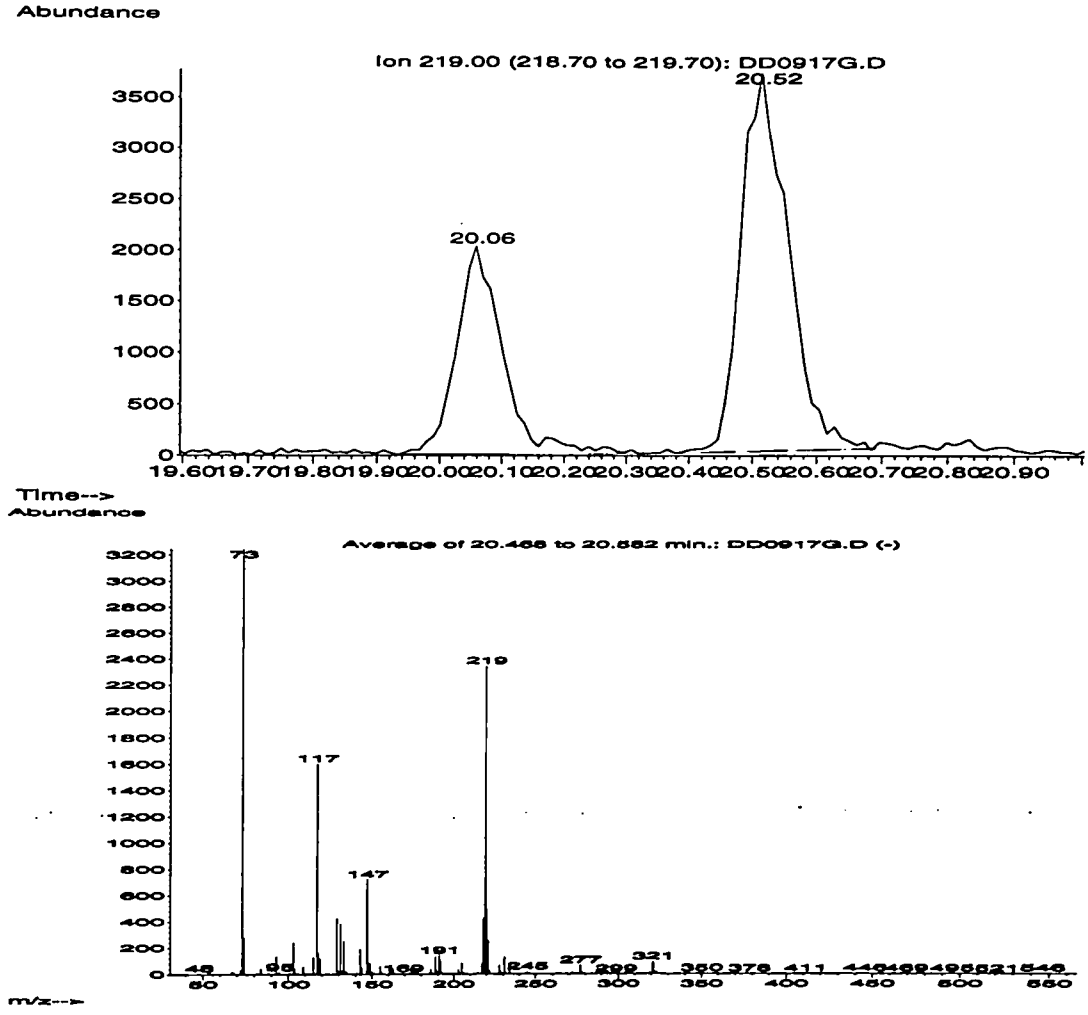


Figure 4-7. Mass chromatogram corresponding to m/z 219 (top) of a derivatized outdoor window sample along with the mass spectrum of the second peak at 20.52 min (bottom).

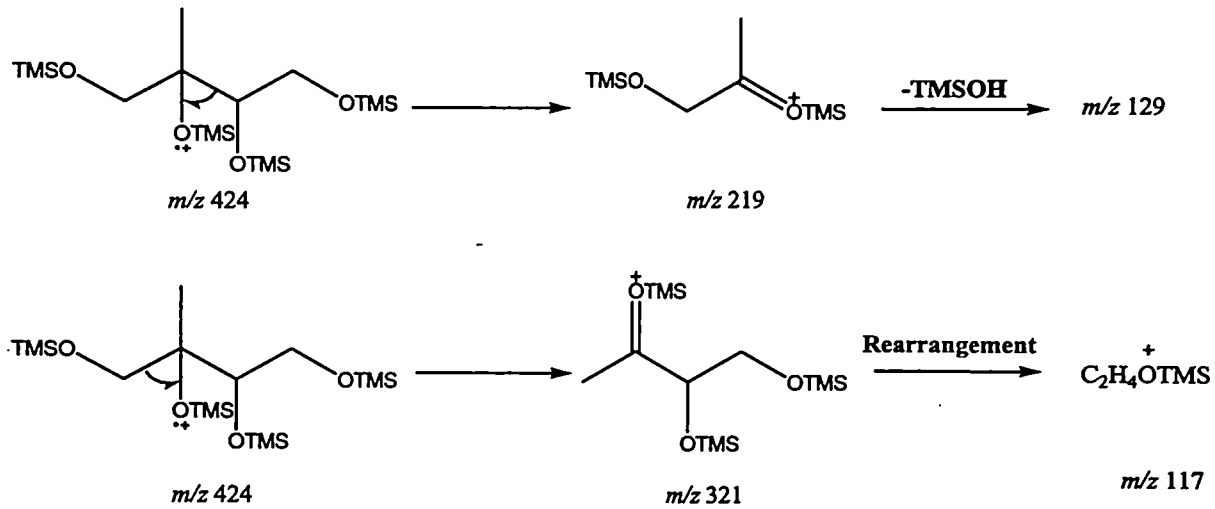


Figure 4-8. Fragmentation pattern of the tetra TMS derivative of 2-methylbutane-1,2,3,4 tetrol as proposed by Claeys et al[38].

4.5 Quantitative Analysis of Analytes Found in the Window Films

4.5.1 Reproducibility of the Results

Quantitation of the analytes was done using deuterated PAH as internal standards (Section 2.6.3). The reproducibility was evaluated on three runs of an outdoor urban restaurant sample (JRO) (Table 4-4). Relative standard deviations of the individual analytes varied from 2-14%. Overall, the total loadings ($\mu g/m^2$) of the analytes had a variability of 6.5%. The assumption was made that all other window film extracts would have similar variabilities as the urban restaurant sample. Since the sample amounts were very small a proper statistical analysis of each sample was not possible.

Table 4-4. Reproducibility of the window film loading (μg/m^2) calculated for identified compounds found in window films of an outdoor urban restaurant sample (JRO)

	1	2	3				
Identified Compound ($MeONH_2$/TMS Derivative)	Urban Restaurant (JRO)	Urban Restaurant (JRO)	Urban Restaurant (JRO)		AVG	STDEV	RSD
Glycerol	3.52	4.06	3.36		3.65	0.37	10.1%
C_5-tetrol	2.14	2.01	1.78		1.98	0.18	9.2%
C_5-tetrol	4.55	3.98	3.54		4.02	0.51	12.6%
Arabinose	4.17	4.56	4.48		4.40	0.21	4.7%
Xylitol	1.28	1.30	1.11		1.23	0.10	8.5%
Levoglucosan	5.13	5.82	5.41		5.45	0.35	6.4%
Pinitol	1.96	1.94	1.75		1.88	0.12	6.2%
L-Quebrachitol	1.21	1.33	1.33		1.29	0.07	5.4%
Fructose	31.8	38.9	35.7		35.5	3.6	10.0%
Glucose	13.6	17.3	14.9		15.3	1.88	12.3%
Myo-Inositol	1.72	1.83	1.77		1.77	0.06	3.1%
Sucrose	13.2	12.7	12.9		12.9	0.25	1.9%
Trehalose	0.587	0.459	0.464		0.50	0.07	14.4%
Stigmastanol	1.3	1.2	1.1		1.20	0.10	8.0%
Total μg/m^2	84.8	96.3	88.4		89.8	5.88	6.5%

4.6 Trends and Patterns in the Window Film Constituents

4.6.1 Indoor vs. Outdoor

In general, the concentrations of the analytes were higher in the outdoor film samples than in indoor samples (Table 4-5 and Figure 4-9).

Table 4-5. Total window film loadings (μg/m^2) of analytes identified in this study. (*URB=average of urban samples, PHW, SR, RS, JR)

Site	OUTDOOR (total μg/m^2)	INDOOR (total μg/m^2)
EB (rural)	173	516
DW (suburban)	316	8.4
*URB	80	39
PHW (urban)	40	18
SR (urban)	119	6.4
RS (urban)	70	46
JR (urban)	91	86

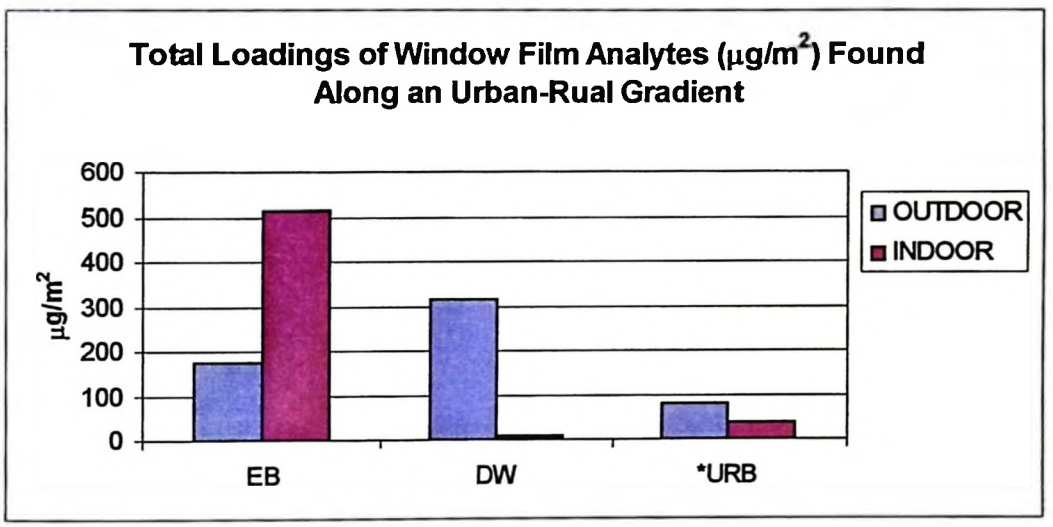


Figure 4-9. Total loadings of window film analytes (μg/m^2) indoor vs. outdoor along an urban-rural gradient.

The exception to this trend was the rural office site (EB). One possibility for a lower concentration of analytes outdoors is that the film is susceptible to wash-off by water and is easily washed away. If it had rained or snowed in Egbert (EB) prior to the sample collection this may have led to lower concentrations outdoors. Since only one rural

sample and one suburban sample were analyzed the true determination of any rural-urban trends may be difficult.

Another observation about the levels of analytes indoors vs. outdoors was noticed at the different types of sites. Figures 4-10, 4-11, and 4-12 shows the concentrations of the positively identified analytes on windows sampled at offices, a lab, a residence and a restaurant. It was interesting to note that at the urban office sites the concentration of analytes was significantly higher outdoor than indoor. At the urban laboratory and urban residence the concentrations outdoor were still larger than indoor, but not by a large amount. Finally, at the rural office and urban restaurant the concentrations outdoor were either similar to or lower than the values indoor. It is possible that the ventilation system in the urban offices is filtering the outdoor air, thereby reducing the amount of saccharides observed indoors. At the other sites indoor activities, such as food cooking, may be contributing to the levels of saccharides indoors.

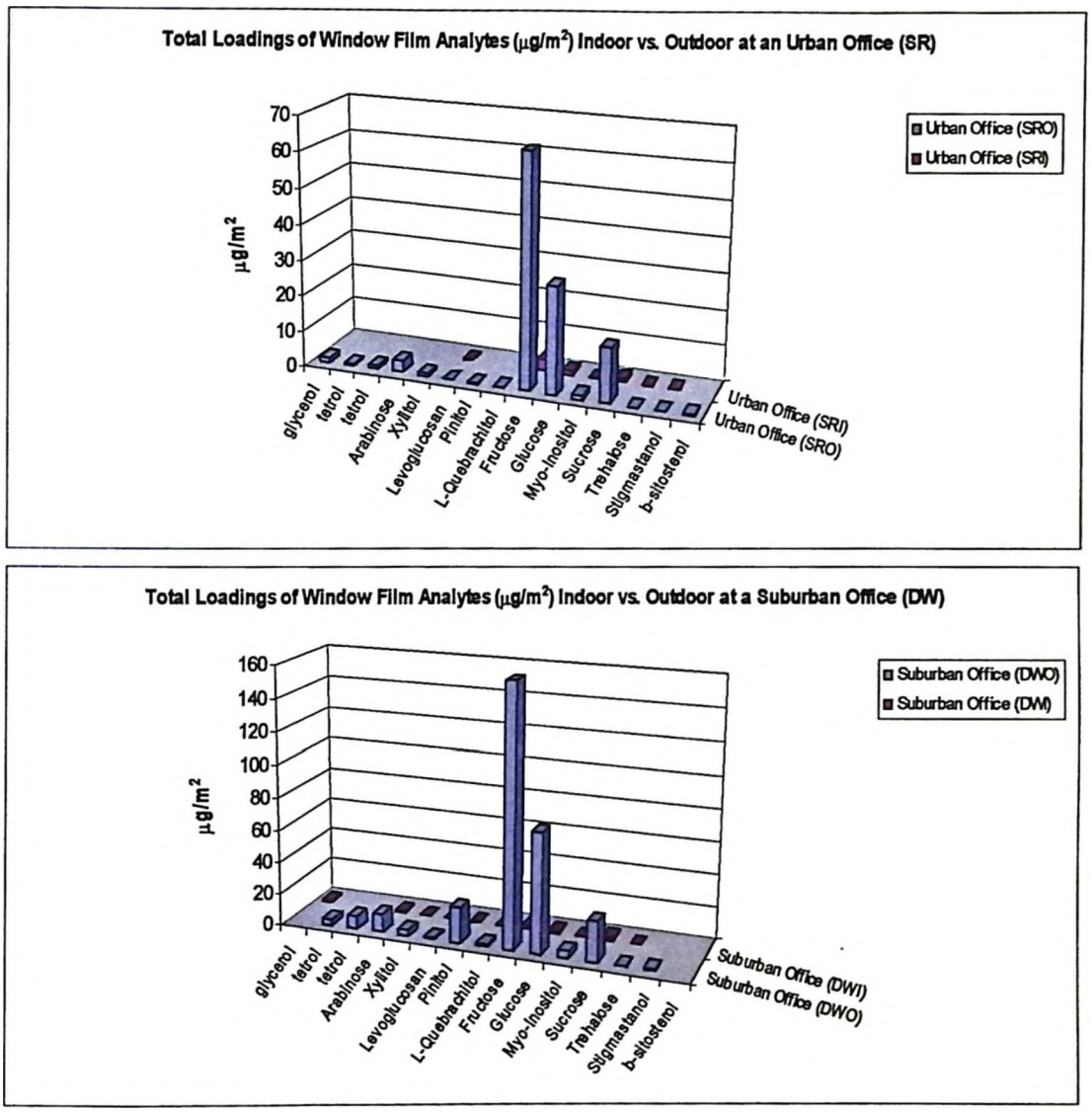


Figure 4-10. Comparison of the loadings of sugars and sugar alcohols (µg/m²) in indoor and outdoor in window films. Similarities about the patterns were observed at the urban office (SR) site and the suburban office (DW) site.

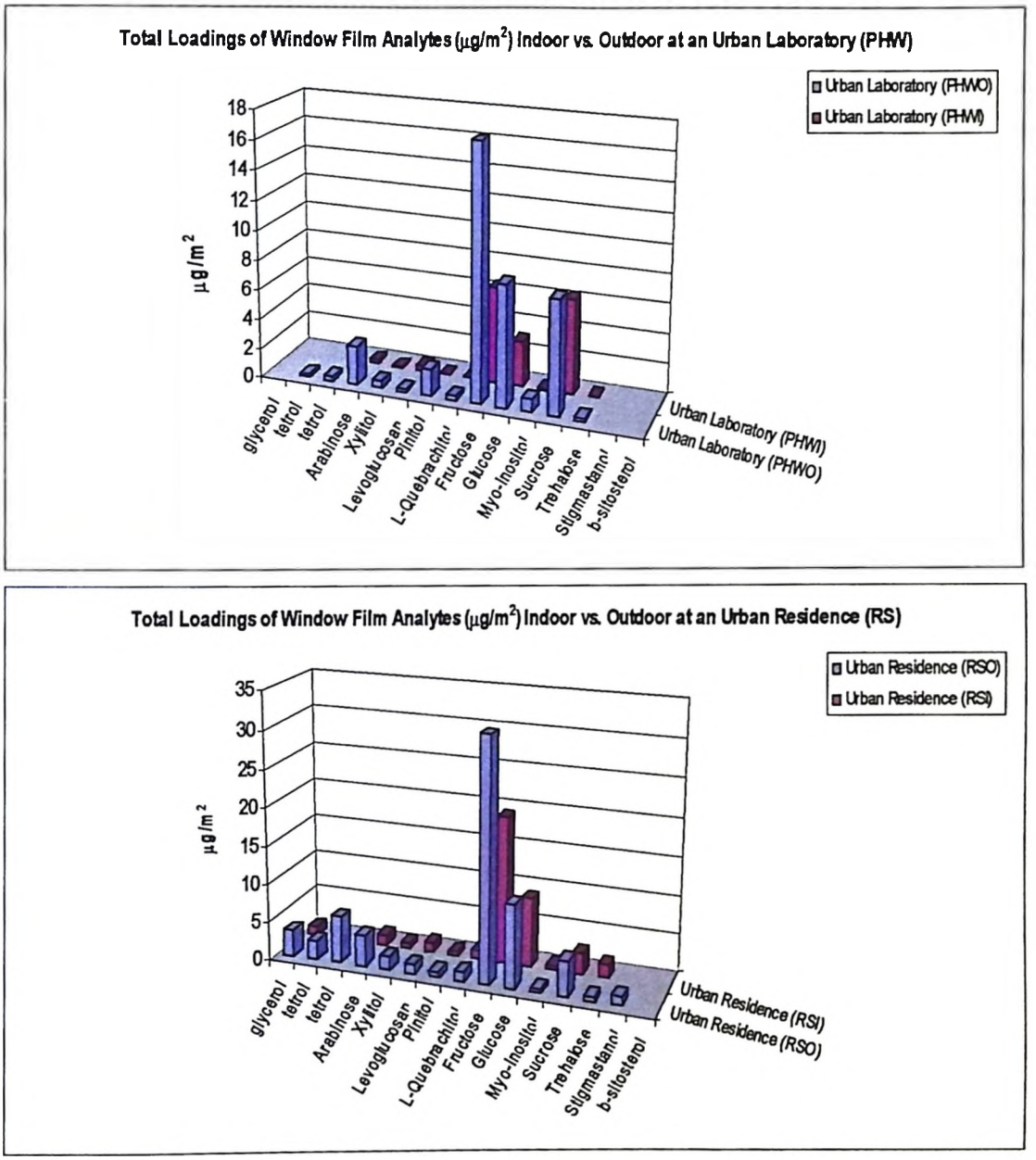


Figure 4-11. Comparison of the loadings of sugars and sugar alcohols (µg/m²) in indoor and outdoor in window films. Similarities about the patterns were observed at the urban laboratory (PHW) site and the urban residence (RS) site.

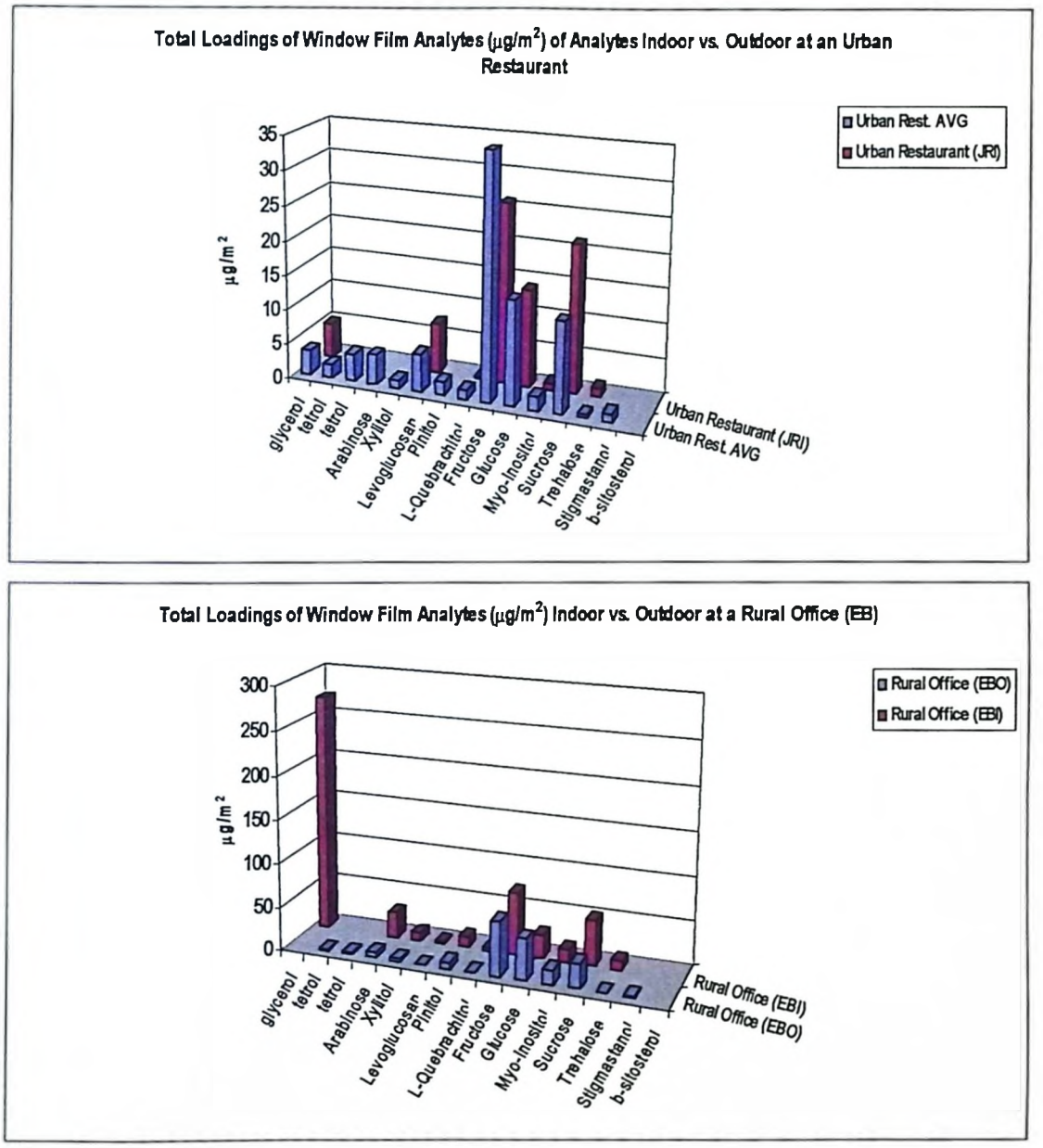


Figure 4-12. Comparison of the loadings of sugars and sugar alcohols (µg/m²) in indoor and outdoor in window films. Similarities about the patterns were observed at the urban restaurant (JR) site and the rural office (EB) site.

4.6.2 Urban vs. Rural

The patterns and distribution of analytes was similar from urban-rural sites with glucose, fructose and sucrose being the most abundant sugars (Figure 4-13). It appeared as though in outdoor samples the order of increasing analyte concentrations went from urban-rural-suburban (Figure 4-9). Indoors the trend was suburban-urban-rural. The percent contribution of the sugars in the window films was consistent when going from urban-rural sites (Figure 4-14a) in outdoor films, while indoor films (Figure 4-14b) showed a lower percent contribution of sugars at the rural site. Percent contributions of sugar alcohols in the outdoor samples (Figure 4-15a) showed that pinitol and myo-inositol were more abundant at the rural site than the urban sites, while the C_5-tetrols were more abundant at urban sites than the rural one. The percent contribution of the sugar alcohols in the indoor window films also showed higher levels of pinitol and myo-inositol at the rural site as well as an abundance of glycerol, which is shown off-scale in Figure 4-15b. Overall, the pattern of sugars found in the window films appears to be fairly consistent when going from urban-rural sites, while the patterns of sugar alcohols seem to vary from urban-rural sites.

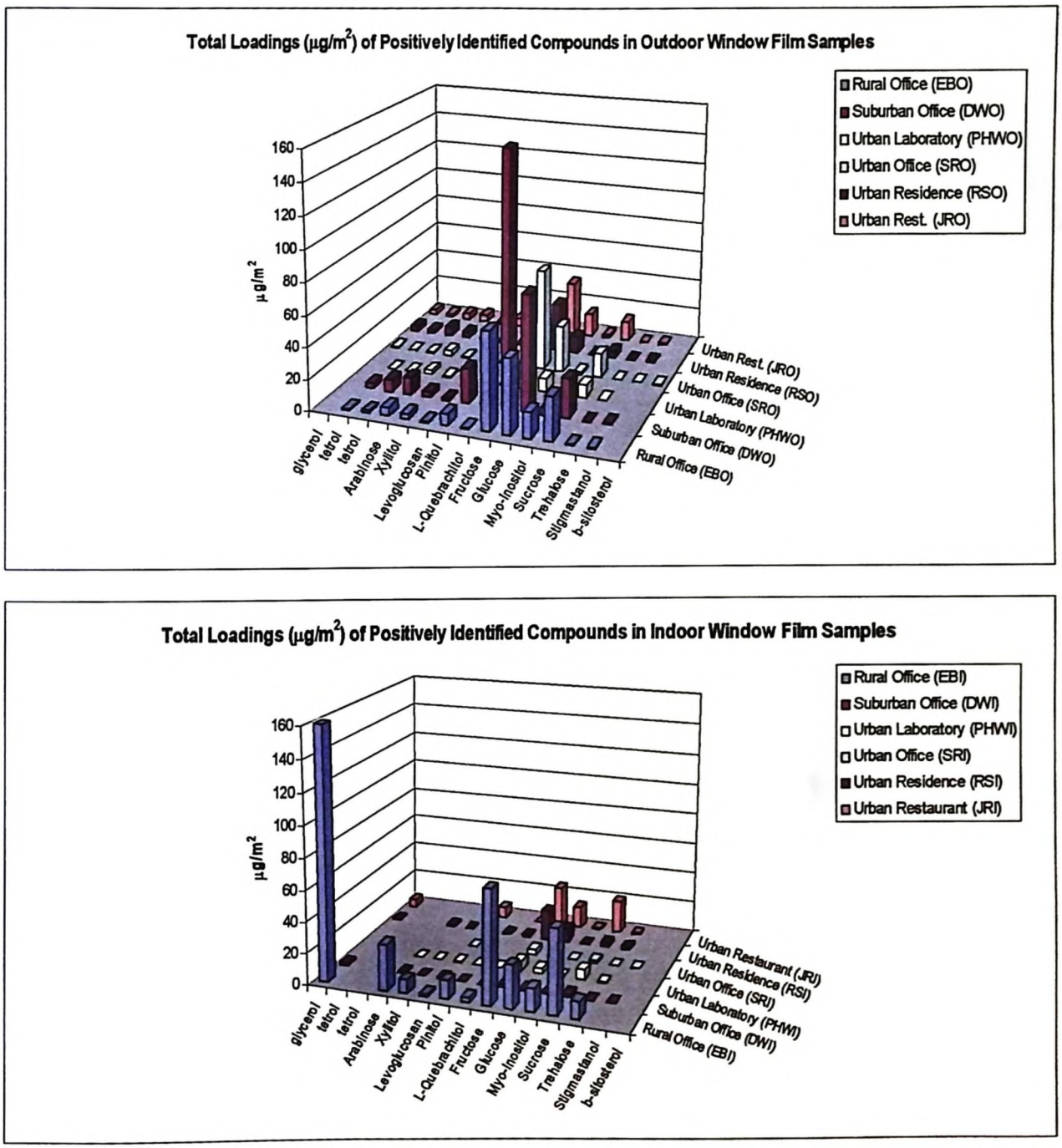


Figure 4-13. Distributions of positively identified compounds found in outdoor window films (top) and in indoor window films (bottom).

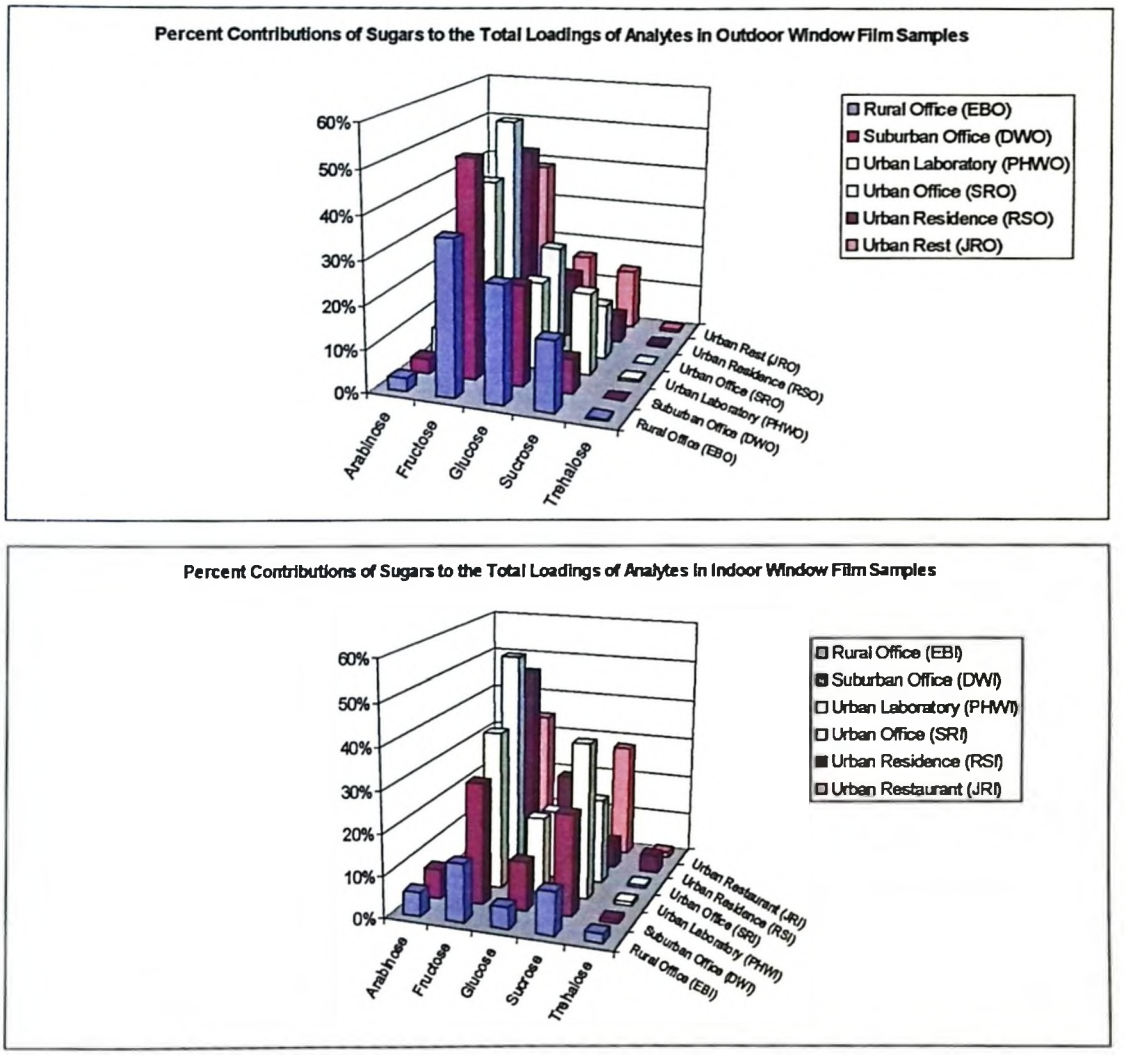


Figure 4-14. Percent contributions of sugars to the total loadings of analytes in outdoor window films (top) and indoor window films (bottom).

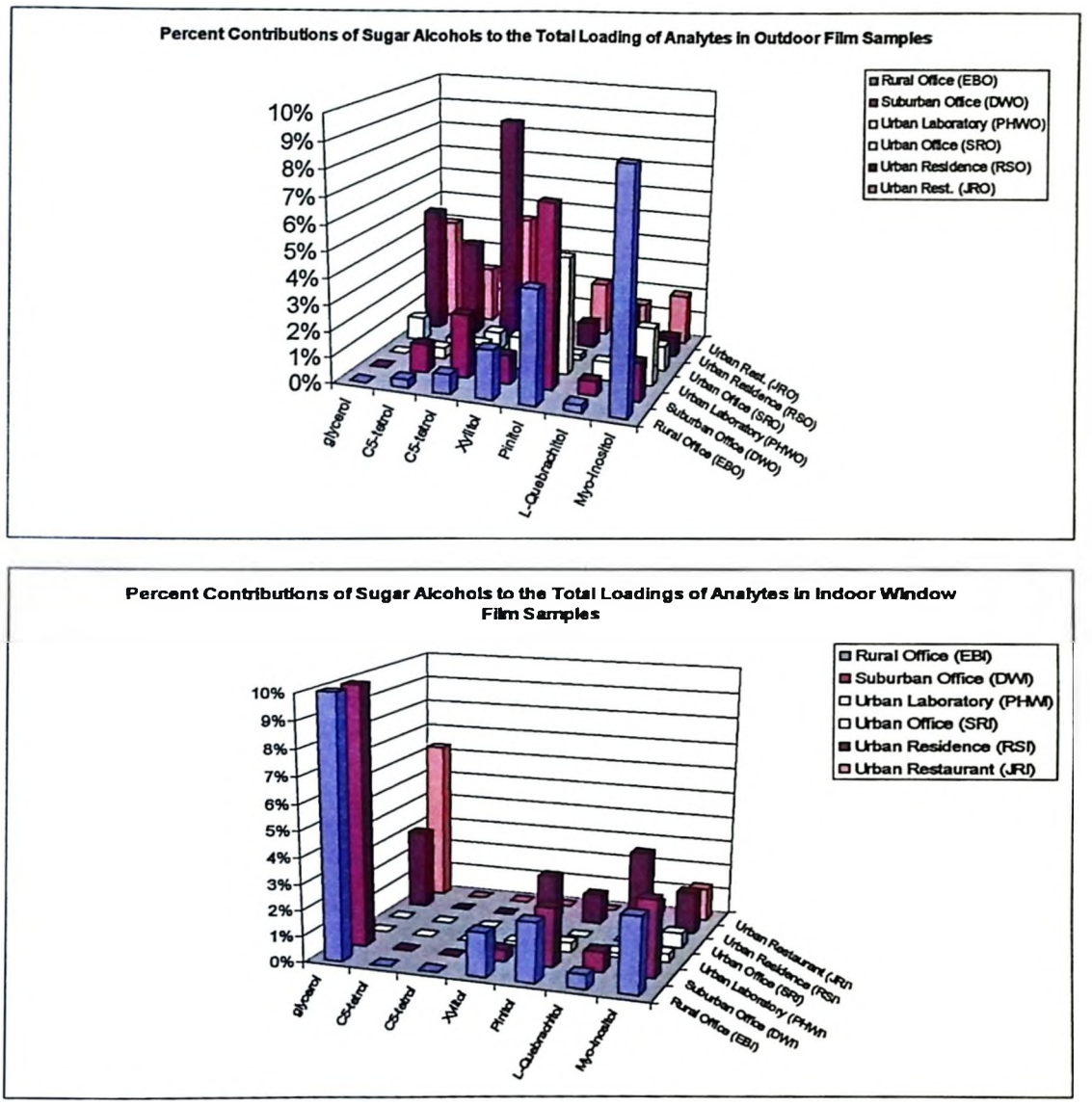


Figure 4-15. Percent contribution of sugar alcohols to the total loadings of analytes in outdoor window films (top) and indoor window films (bottom).

4.7 Comparison of Compositions of Window Film Samples to Air Particulate Material

Air particulate samples that had been collected in July 1995 at two different sites in Hamilton, ON were extracted using Soxhlet extraction with dichloromethane (12 hours) then methanol (12 hours). Only the methanol extract was derivatized using the method with $MeONH_2 \cdot HCl$/pyridine then MSTFA. The sampling sites were in the very east end of Hamilton at Pier 25 (PM_{10}) and Philip Environmental (PM_{10} and TSP). Approximately 1600 m^3 of air was collected over 24 hours and the methanol extracts were made up to 10 mL, resulting in solutions containing the equivalent of 0.16 $m^3/\mu L$. A 10 µL aliquot (equivalent to 1.6 m^3) was evaporated to dryness, derivatized and made up to a final volume of 10 µL. A 1 µL aliquot was injected onto the GC/MS, corresponding to 0.16 m^3 of sample. Positive identifications for analytes in the aerosol samples had to meet the same criteria as the window film samples (Section 4.1). Many of the sugars and sugar alcohols identified in the Toronto window film samples were observed in the Hamilton aerosol samples. In the aerosol samples the major differences were the lack of arabinose, L-quebrachitol, myo-inositol and the abundance of mannitol rather than fructose (figure 4-16b). None of the plant sterols were detected in the aerosol samples. Figure 4-16a depicts typical total ion chromatograms from aerosol samples and window film samples.

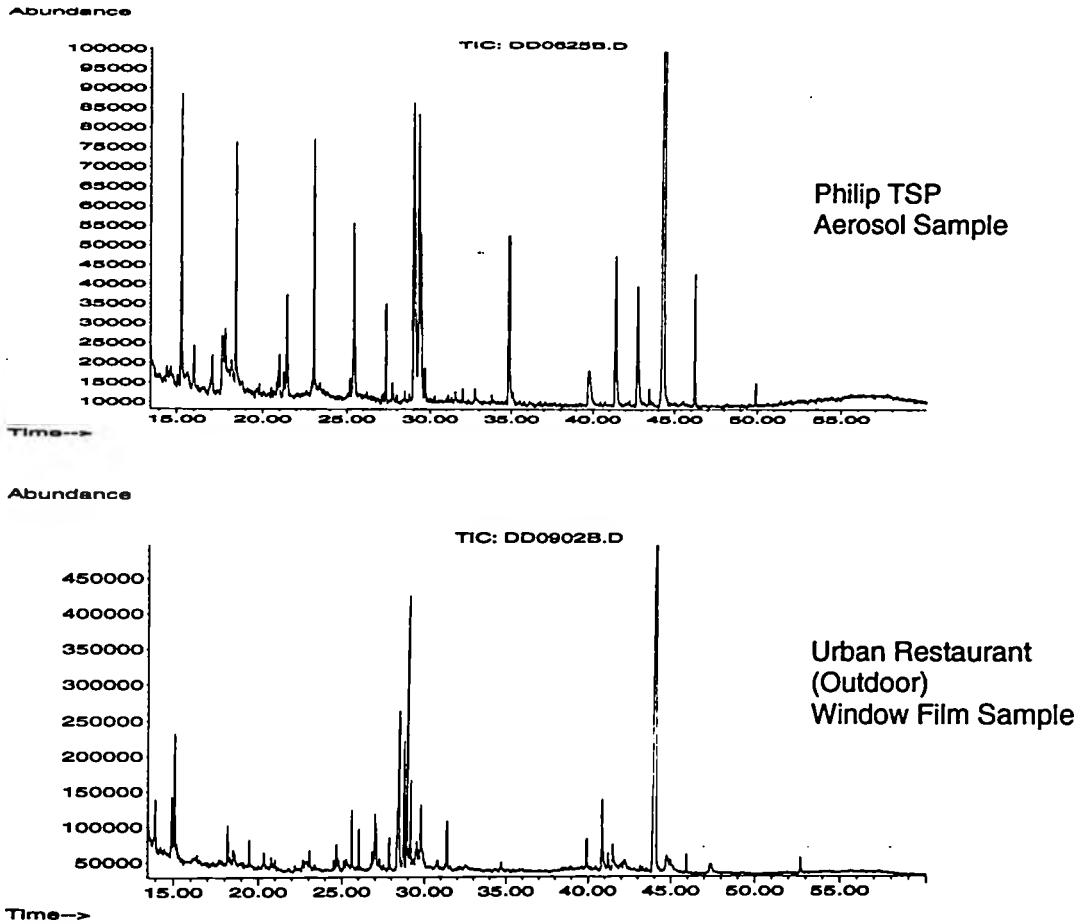


Figure 4-16a. Total ion chromatograms of a typical aerosol sample (Philip TSP) and a typical window film sample (urban restaurant).

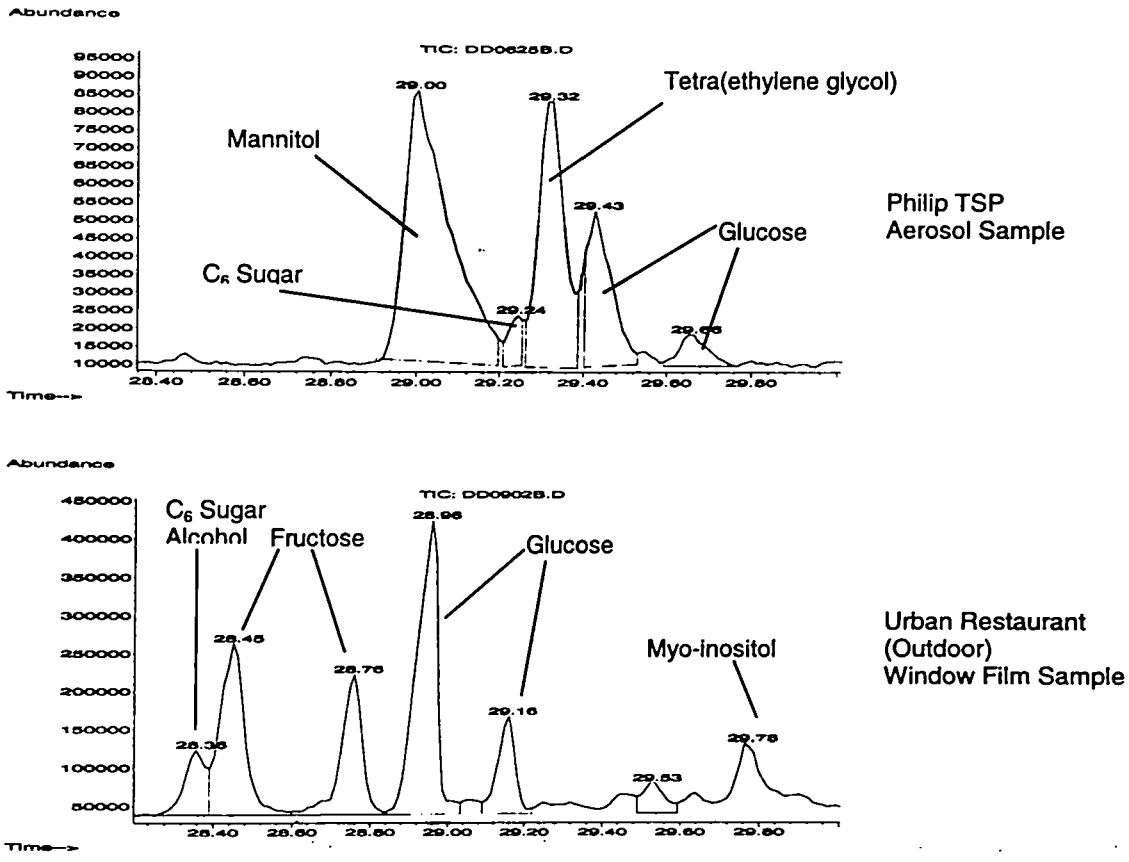


Figure 4-16b. Differences between the sugars observed in the aerosol samples and window film samples in the region of 28.4 min. to 30 min.

Mannitol is the sugar alcohol form of fructose. Bacteria, such as the Leuconostoc bacteria found in nature, contains the enzyme mannitol dehydrogenase which can reduce fructose to mannitol[43-45]. The other possibility is that the source(s) of mannitol in the aerosol samples and the source(s) of fructose in the window films are different.

By dividing the peak area of each analyte by the total peak area in the total ion chromatogram, the percentage contribution of each peak could be determined (Table 4-6). The distribution of sugars found in the aerosol samples resembles those found in window films (Figure 4-17).

4.7.1. Aerosols collected in Hamilton, ON Canada Compared to Other Areas

The levels of the various sugars (ng/m^3) detected in the Hamilton aerosol samples were compared to values found in aerosols in the literature (Table 4-7). It is difficult to make comparisons between the samples since many of the samples were collected in different environments and during different seasons. Aerosol samples from Chile, Malaysia, Japan and China were all collected over the Pacific Ocean[21]. The Belgian[7] and USA[88] samples were collected in urban areas, while the Brazil aerosols were collected in the Brazilian Amazon region[23]. The Pier 25 and Phillips samples are unusual in that they were collected in industrial areas rather than in urban or rural areas. The most common sugars present at each of the locales were levoglucosan, glucose, sucrose and trehalose (mycose).

Table 4-6. Percent contributions of the peaks identified in the total peak area in the total ion chromatogram for aerosol samples (top) and outdoor window film samples (bottom).

Aerosol ($MeONH_2$/TMS Derivative)	Philip PM10	Philip TSP	Pier 25 PM10
C_5-tetrol	3.1	3.3	4.4
C_5-tetrol	6.3	6.9	7.5
Arabinose	0	0	0
Xylitol	5.0	9.8	9.3
Levoglucosan	1.8	2.9	3.2
Pinitol	0.8	1.0	1.5
L-Quebrachitol	0	0	0
Mannitol	14	23	21
Fructose	0	0	0
Glucose	5.6	9.2	11
Sucrose	2.4	11	3.3
Trehalose	2.8	8.6	8.5

Window Film ($MeONH_2$/TMS Derivative)	EBO	DWO	PHWO	SRO	RSO	JRO
C_5-tetrol	0.3	0.9	0	0.2	1.6	1.3
C_5-tetrol	1.7	1.1	0	0.2	1.6	0.9
Arabinose	3.0	1.6	5.5	2.1	3.3	2.8
Xylitol	2.3	1.6	2.0	1.1	4.1	2.0
Levoglucosan	0.6	0.3	0.4	0.4	1.2	3.9
Pinitol	2.9	6.8	3.6	0.4	0.9	2.3
L-Quebrachitol	0.3	0.6	0.7	0.3	1.9	1.1
Mannitol	0	0	0	0	0	0
Fructose	28	32	22	36	27	23
Glucose	32	33	26	31	24	22
Myo-Inositol	8.2	1.8	2.3	1.4	1.1	2.5
Sucrose	11	9.7	23	14	9.3	14
Trehalose	0.6	0.1	0.7	0.5	2.0	1.8

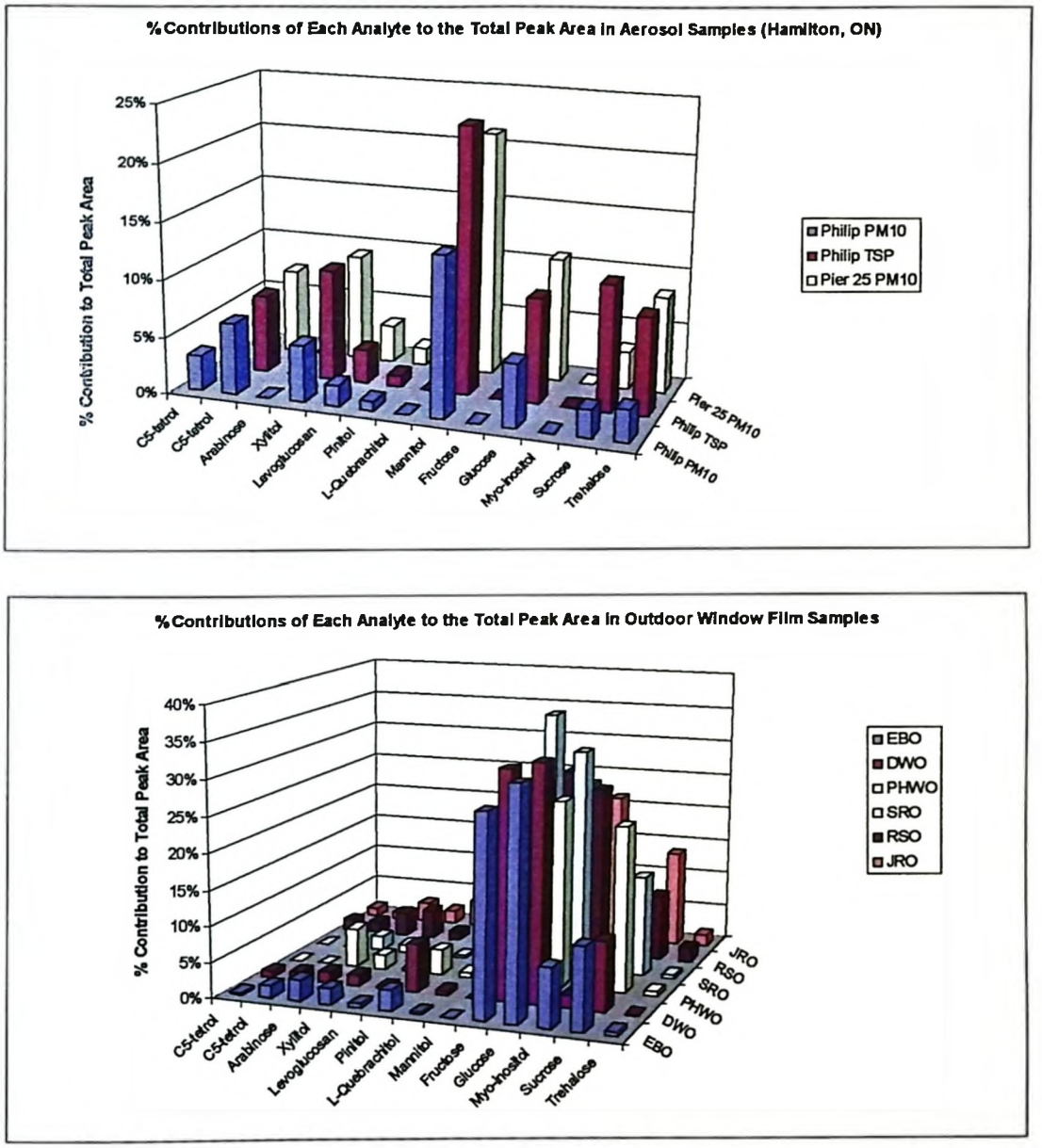


Figure 4-17. Percent contributions of sugars and sugar alcohols to the total peak area in aerosol samples (top) and outdoor window film samples (bottom).

Table 4-7. Comparison of concentrations (ng/m^3) of sugars and sugar derivatives found in aerosol samples collected at various locales.

	Hamilton, ON Canada										
Compound	Philips PM_{10}	Philips TSP	Pier 25 PM_{10}	Balbina, Brazil[37] (PM2.5, TSP)	Santiago, Chile[20] (TSP)	Kuala Lumpur, Malaysia[21] (TSP)	Sapporo, Japan[21] (TSP)	Ghent, Belgium[7] (PM_{10})	Rondonia, Brazil[23] (PM_{10} & $PM_{2.5}$)	Various Locales, USA[88]	Datong, P.R. China[21] (TSP)
Glycerol	n.d.	n.d.	n.d.				3-24		0.5-9		
C_5-tetrol (erythro & threo)	74	84	98	41-65							
Erythritol	n.d.	n.d.	n.d.						2-39		
Xylitol	7	16	15				2-22				
Xylose	n.d.	n.d.	n.d.						1-33	9-17	
Levoglucosan	4	10	9	12-38	12-2452	1162-33400	6-56	121-1133	1182-6900	500-2980	1350
Mannosan	n.d.	n.d.	n.d.		1-233	154-4430	0.2-15	17-153	6-371	170-322	108
Galactosan	n.d.	n.d.	n.d.		1.7-127	84-2410	0.6-2.4	4-44	2-148	96-144	106
Inositols	1	2	1				3-104		0.5-21		
Mannitol	6	14	13	8-68					10-50		
Mannose	n.d.	n.d.	n.d.			48-6800			0.6-4	9-13	
1,6-anhydroglucofuranose	n.d.	n.d.	n.d.		0.5-195	135-4005			5-248		
Fructose	n.d.	n.d.	n.d.				12		3-20		
Glucose	7	16	12	0.6-134	10-2210		1-34		14-62	10-15	102
Galactose	n.d.	n.d.	n.d.						0.2-2.4		
Sorbitol	n.d.	n.d.	n.d.				3-26		0-1.7		
Sucrose	5	28	7		15-3060		0.4-9		0.8-26	3.2-4	1148
Maltose	n.d.	n.d.	n.d.		6-2390	2-550				3-4	68
Mycose	4	13	12		8-1660		0.2-12		5-18		54

n.d. = not detected

4.8 Kimwipe Blanks

One concern about the identification of sugars in these samples was that they may have arisen as artifacts from the Kimwipes used. Since the Kimwipes had only been cleaned with dichloromethane prior to sampling, the sugars and sugar alcohols could have come from the wood fiber that makes up the Kimwipes. Field blanks from the urban restaurant were available for the outdoor samples and field blanks from an urban residence were available for the indoor samples. Field blanks in this study were lab tissues (pre-cleaned with DCM only) that were taken into the field and then shaken in the air to simulate exposure during sampling. The blanks were subjected to the same derivatization procedure as the sample extracts. Detectable, but low levels of arabinose, levoglucosan, pinitol, L-quebrachitol, glucose and sucrose were detected in the field blanks for the outdoor samples (Table 4-8). A different number of Kimwipes were used to collect the samples at each site so the $\mu g/m^2$ values were converted to μg/Kimwipe (KW). Arabinose had a maximum contribution of 8%, while the other compounds contributed less than 5%. In the indoor samples no saccharides were detected in the field blank.

Table 4-8. Loadings (μg/KW) of sugars and sugar alcohols found in the field blanks compared to the loadings (μg/KW) found in outdoor window film samples. (%=Percent contribution of field blanks to the sample)

Compound ($MeONH_2$/TMS Derivative)	Field Blanks (μg/KW)	EBO (μg/KW)	%	DWO (μg/KW)	%	PHWO (μg/KW)	%
Arabinose	0.08	3	3%	8	1.0%	0.9	8%
Levoglucosan	0.003	0.2	2%	0.7	0.4%	0.07	4%
Pinitol	0.003	4	0.1%	16	0.02%	0.6	0.5%
L-Quebrachitol	0.004	0.2	2%	1	0.4%	0.09	4%
Glucose	0.03	20	0.2%	53	0.1%	3	1%
Sucrose	0.007	2	0.4%	18	0.04%	3	0.2%
Compound ($MeONH_2$/TMS Derivative)	Field Blanks (μg/KW)	SRO (μg/KW)	%	RSO (μg/KW)	%	JRO (μg/KW)	%
Arabinose	0.08	1	8%	2	4%	1	8%
Levoglucosan	0.003	0.1	3%	0.5	1%	2	0.2%
Pinitol	0.003	0.1	3%	0.3	1%	0.6	1%
L-Quebrachitol	0.004	0.07	6%	0.6	1%	0.4	1%
Glucose	0.02	13	0.2%	5	0.4%	5	0.4%
Sucrose	0.007	6	0.1%	2	0.4%	4	0.2%

4.9 Summary of Results

Relative to the previous target analytes identified in the window films (alkanes, alkanoic acids, alkanoic diacids, aromatic acids and resin acids), the sugars and sugar alcohols constitute 55-99% of the total $\mu g/m^2$ of identified compounds (Table 4-9). Simoneit reported that saccharides comprise 13 to 26% of the total compound mass (TCM) in aerosols[19], and over the ocean up to 63%[21].

Table 4-9. Percent contributions of sugars and sugar alcohols to the total loadings ($\mu g/m^2$) of identified compounds thus far in the window film samples.

	OUTDOOR Loadings ($\mu g/m^2$)			
	Sugars, Sugar Alcohols	Alkanes, Alkanoic acids, Alkanoic Diacids, Aromatic Acids, Resin Acids[1]	Total ($\mu g/m^2$)	% Contribution of Sugars/Sugar Alcohols to Total
EB	173	1	174	99%
DW	316	15	331	95%
PHW	40	33	73	55%
SR	119	17	136	88%

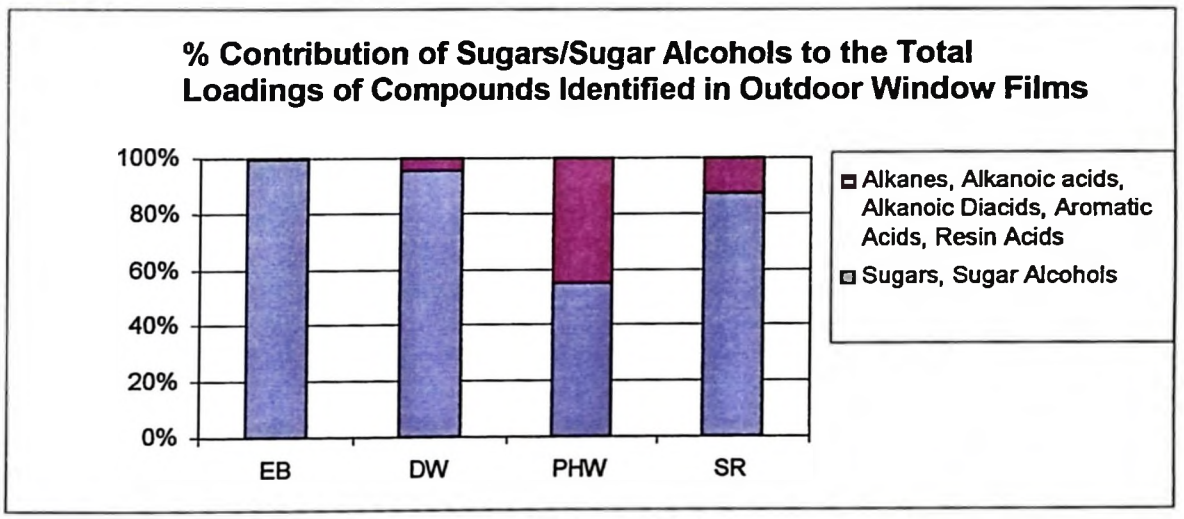


Figure 4-18. Percent contributions of sugars/sugar alcohols to the total loadings of identified compounds thus far in the window film samples.

4.10 Conclusions and Future Work

In conclusion a number of new compounds have been observed in the methanol extracts of window film samples; these compounds were mainly sugars and sugar alcohols. It is highly likely that these water-soluble polar compounds contribute significantly to the indiscriminant wash-off of the film from impervious surfaces. However, more work needs to be done on the bulk characterization of the organic window film.

As mentioned in the introduction (Section 1.8) humic-like substances (HULIS) have recently been reported as being significant components in the water soluble organic carbon (WSOC) fraction of aerosol samples[87]. It is likely that similar compounds would therefore exist in the window films. In order to analyze for these high molecular weight compounds LC/MS should be used. More structural information could be provided using LC/MS/MS on a triple quadrupole mass spectrometer and higher resolution could be achieved using a LC system coupled to a quadrupole-time-of-flight (Q-TOF) instrument.

Further sampling could also be done at both urban and rural sites. Simultaneous sampling of air (both gas-phase and particle-phase) and film would give a better picture of the contribution that the particle-associated organics make to the organic components in the film. Additionally, the film samples could be collected on small glass panes rather than on windows. By using small panes of glass the samples can be collected in "protected" and "unprotected" settings. The "protected" samples would be exposed to the ambient air, but not to rain, which would result in no wash-off. The "unprotected" samples would be exposed just like a regular window. Sampling over different periods

(e.g. 1 day, 2 days, 1 week, 2 months etc...) would allow us to monitor the rate of build-up of the film over time. Atomic force microscopy (AFM) would also allow us to monitor the rate of build-up on the film and to also characterize the film.

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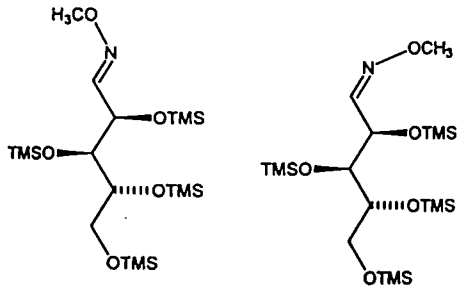
6.0 APPENDICES

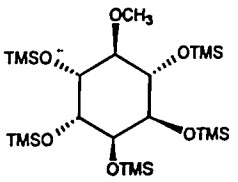
Appendix 1

Structures of derivatized compounds observed in the methanol extracts of organic window films.

Appendix 1. Structures of derivatized compounds observed in the methanol extracts of organic window films.



Arabinose MEOX $(TMS)_4$



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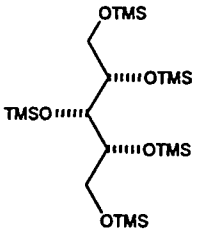

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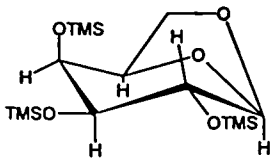
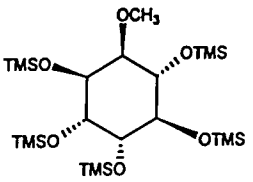
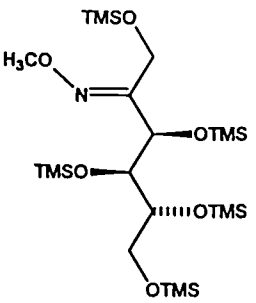
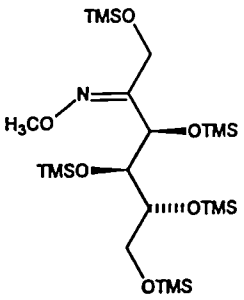


Levoglucosan $(TMS)_3$

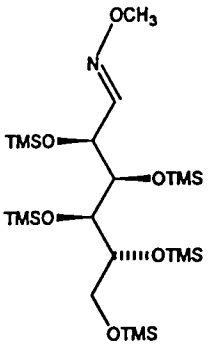


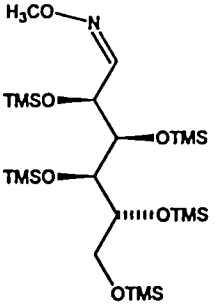
L-Quebrachitol $(TMS)_5$



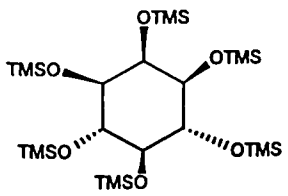


Fructose MEOX $(TMS)_5$

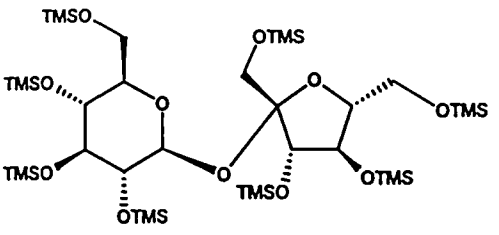




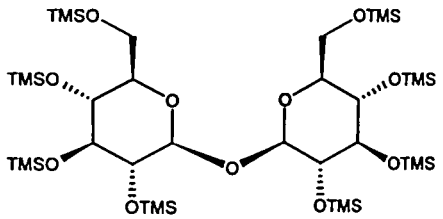
Glucose MEOX $(TMS)_5$



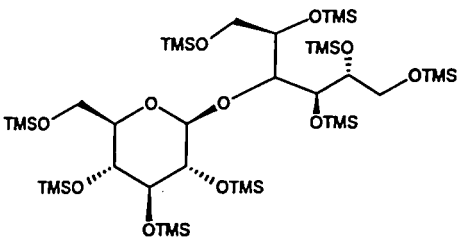
Myo-Inositol $(TMS)_6$



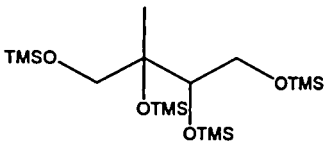
Sucrose $(TMS)_8$



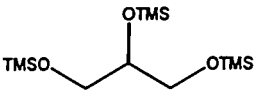
Trehalose $(TMS)_8$



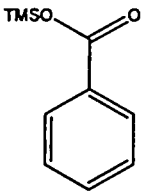
Maltitol $(TMS)_9$



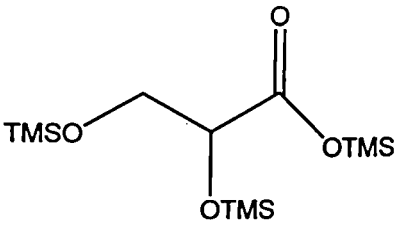
C_5-Tetrol $(TMS)_4$
(erythro & threo)



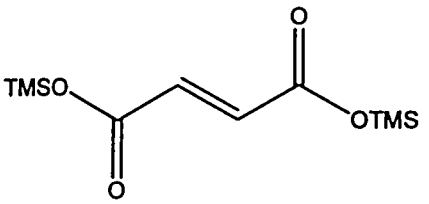
Glycerol $(TMS)_3$



Benzoic Acid (TMS)



Glyceric Acid $(TMS)_3$



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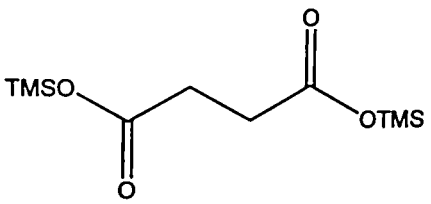
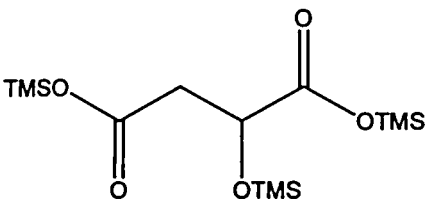


Succinic Acid $(TMS)_2$



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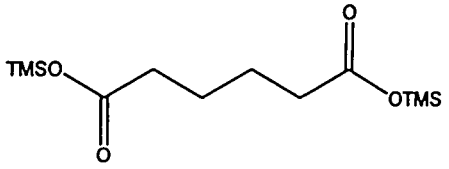
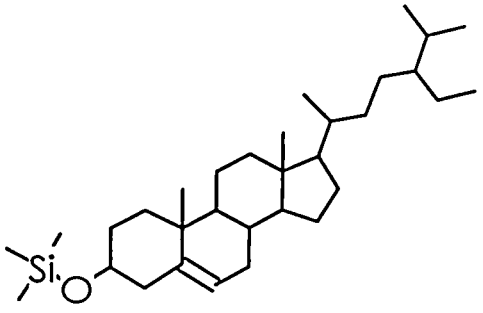
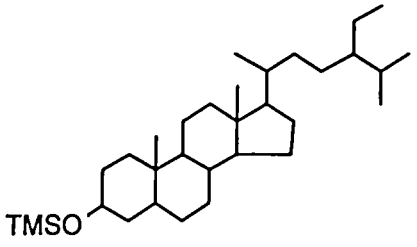


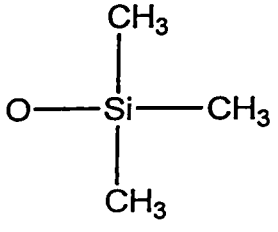
Adipic Acid $(TMS)_2$



β-Sitosterol (TMS)



Stigmastanol (TMS)

OTMS = 

Appendix 2

Retention Index Values of Positively Identified, Tentatively* Identified and Unknown** Compounds Observed in Methanol Extracts of Window Film Samples.

*Tentatively Identifed Compounds are shown in brackets
**Unknown compounds are shown by blank spaces

		Outdoor Window Films						Indoor Window Films									
	Compound	EBO	DWO	PHWO	SRO	RSO	JRO	EBI	DWI	PHWI	SRI	RSI	JRI	AVG	STDEV	# Outdoor	# Indoor
1											715.9		715.5	715.7	0.3	0	2
2										719.2				719.2	-	0	1
3						724.7			727.6	728.0	729.3	728.5	730.5	728.1	-	1	5
4				735.6										735.6	-	1	0
5	glycerol				765.3	766.9	764.4	770.3	769.0			771.1	766.1	767.6	2.6	3	4
6					777.8									777.8	-	1	0
7	glycine											812.6		812.6	-	0	1
8										834.7				834.7	-	0	1
9					856.5					852.3	849.4			852.7	3.6	1	2
10	glyceric acid								869.0			865.7		867.4	2.4	0	2
11										876.2	876.6		876.2	876.3	0.2	0	3
12								770.3						770.3	-	0	1
13	benzoic acid							864.9						864.9	-	0	1
14	glyceric acid							869.0						869.0	-	0	1
15									877.0					877.0	-	0	1
16	fumaric acid							889.1						889.1	-	0	1
17	succinic acid							903.6	902.2	902.7	902.7	903.1	902.2	902.7	0.5	0	6
18											907.6			907.6	-	0	1
19										912.4	912.9	913.7		913.0	0.7	0	3
20								928.6						928.6	-	0	1
21							965.3	968.5	967.0					966.9	1.6	1	2
22												979.4		979.4	-	0	1
23									986.7		992.2	992.2		990.4	3.2	0	3
24	(C_4 sugar)		993.3											993.3	-	1	0
25												997.6		997.6	-	0	1
26								997.5		997.6	997.6			997.6	0.0	0	3
27	C_5-tetrol	999.8	1000.9	1002.4	997.3	998.2	991.1							998.3	4.0	6	0
28								1000.2						1000.2	-	0	1
29	C_5-tetrol	1019.1	1020.1	1021.1	1017.3	1017.3	1011.1							1017.7	3.5	6	0
30										1014.0				1014.0	-	0	1
31			1024.2		1021.3	1028.4	1024.4				1025.2			1024.7	2.5	4	1
32	malic acid							1057.5				1057.9		1057.7	0.3	0	2
33			1073.2					1075.4						1074.3	1.5	1	1
34						1097.3					1095.1			1096.2	1.6	1	1
35	adipic acid							1107.7	1106.3			1107.2	1105.8	1106.8	0.9	0	4
36		1113.5	1113.5		1113.9	1113.5	1114.9							1113.9	0.6	5	0

	Compound	EBO	DWO	PHWO	SRO	RSO	JRO	EBI	DWI	PHWI	SRI	RSI	JRI		AVG	STDEV	# Outdoor	# Indoor
37						1116.4				1116.9		1116.9			1116.7	0.3	1	2
38												1136.1	1136.1		1136.1	0.0	0	2
39								1157.3				1162.2			1159.8	3.4	0	2
40								1178.6							1178.6	-	0	1
41								1186.7							1186.7	-	0	1
42	arabinose	1192.8	1191.8	1194.0	1189.4	1190.8	1186.3	1192.5	1193.7	1193.5		1192.0			1191.7	2.4	6	4
43			1194.7			1194.7									1194.7	0.0	2	0
44	glutamine										1197.8	1197.8	1197.3		1197.7	0.3	0	3
45	arabinose	1200.5	1200.5	1201.7	1198.1	1199.0	1194.0	1200.7	1201.4	1202.2		1200.2			1199.8	2.4	6	4
46											1207.0		1207.5		1207.2	0.3	0	2
47	(sugar alcohol)			1208.0											1208.0	-	1	0
48	xylitol	1209.7	1208.2	1213.3	1205.8	1206.8	1197.8	1210.4	1213.5	1209.9		1209.9			1208.5	4.5	6	4
49							1217.6				1215.7				1216.6	1.4	1	1
50							1222.4								1222.4	-	1	0
51								1231.6							1231.6	-	0	1
52							1258.6								1258.6	-	1	0
53								1264.8		1266.7			1267.2		1266.3	1.3	0	3
54	(C_6 Sugar Alcohol)	1279.2	1278.3	1282.2				1279.8		1280.2		1282.7	1307.4		1284.2	10.3	3	4
55	levoglucosan	1307.9	1307.9	1308.4	1306.3	1307.9	1307.4	1308.9	1306.8	1307.3	1307.3	1307.9			1307.6	0.7	6	5
56	pinitol	1319.9	1318.8	1321.5	1315.7	1317.9	1311.1	1321.0	1323.6	1320.4		1318.4			1318.8	3.5	6	4
57			1326.7		1324.7	1325.8	1322.6			1327.2					1325.4	1.8	4	1
58		1339.4	1338.7	1340.8	1337.3	1338.9	1335.3	1334.6		1339.3					1338.0	2.1	6	2
59								1350.9							1350.9	-	0	1
60	L-quebrachitol	1359.8	1359.7	1361.8	1355.6	1358.9	1352.6	1361.4	1363.5	1360.2		1359.3	1361.6		1359.5	3.0	6	5
61	(sugar alcohol)	1380.3	1379.1	1381.7	1377.7	1380.0	1376.8	1378.7				1377.2			1378.9	1.7	6	2
62	fructose	1389.2	1390.1	1388.5	1388.7	1386.3	1382.6	1389.8	1390.3	1386.9	1389.2	1387.1	1388.9		1388.1	2.1	6	6
63	(C_6-sugar)	1392.9	1393.2	1392.1	1391.3	1391.6	1392.6	1397.6	1397.1	1399.5	1395.5	1391.3	1396.8		1394.3	2.9	6	6
64	fructose	1405.0	1404.7	1403.7	1403.9	1402.6	1398.9	1405.5	1405.5	1402.6	1405.5	1403.4	1404.2		1403.8	1.9	6	6
65	azelaic acid							1412.3							1412.3	-	0	1
66	glucose	1416.5	1418.3	1413.6	1418.6	1413.2	1409.5	1414.4	1415.0	1413.1	1413.9	1413.9	1414.2		1414.5	2.5	6	6
67	glucose	1426.0	1427.7	1425.1	1427.0	1423.7	1420.0	1425.5	1427.0	1423.6	1426.0	1424.9	1425.8		1425.2	2.1	6	6
68								1445.4							1445.4	-	0	1
69								1452.2							1452.2	-	0	1
70		1493.7			1492.1										1492.9	1.1	2	0
71	(inositol)	1508.2				1509.4									1508.8	0.8	2	0

	Compound	EBO	DWO	PHWO	SRO	RSO	JRO	EBI	DWI	PHWI	SRI	RSI	JRI	AVG	STDEV	# Outdoor	# Indoor
72			1509.4											1509.4	-	1	0
73										1530.4				1530.4	-	0	1
74			1534.8		1534.2					1534.5	1532.1		1532.0	1533.5	1.3	2	3
75										1538.7				1538.7	-	0	1
76	myo-Inositol	1549.5	1550.7	1553.6	1547.1	1551.8	1541.2	1550.7	1554.2	1551.8	1554.7	1551.0	1551.6	1550.7	3.6	6	6
77					1569.5									1569.5	-	1	0
78	hexadecanoic acid							1605.5	1605.4	1604.8	1605.2	1605.6	1605.6	1605.4	0.3	0	6
79							1666.1				1658.1			1662.1	5.7	1	1
80	octadecanoic acid							1807.6	1805.4	1805.4	1805.5	1805.0	1805.0	1805.7	1.0	0	6
81										1965.7				1965.7	-	0	1
82				1982.7	1980.7			1987.1	1987.5	1985.3		1985.6		1984.8	2.6	2	4
83								2000.9						2000.9	-	0	1
84										2056.3				2056.3	-	0	1
85	sucrose	2139.3	2140.0	2137.3	2137.9	2137.3	2131.1	2145.6	2143.4	2139.6	2143.0	2139.7	2138.5	2139.4	3.7	6	6
86							2144.8							2144.8	-	1	0
87		2156.4	2155.0	2154.4	2156.4	2156.4	2156.4							2155.8	0.9	6	0
88					2163.9									2163.9	-	1	0
89								2182.7				2177.8	2177.7	2179.4	2.9	0	3
90	(disaccharide)							2197.1	2188.5	2176.1		2192.0		2188.4	8.9	0	4
91	(disaccharide)		2205.0				2208.4	2204.6				2198.8		2204.2	4.0	2	2
92	(disaccharide)		2213.2		2210.4		2215.2	2218.4		2212.0		2213.8		2213.8	2.7	3	3
93	(disaccharide)				2220.0			2230.0		2222.2				2224.1	5.3	1	2
94	trehalose	2231.6	2230.3	2233.7	2228.2	2231.6	2223.4	2236.9	2239.1	2228.3	2231.1	2230.7	2229.7	2231.2	4.1	6	6
95										2248.6				2248.6	-	0	1
96	(disaccharide)	2265.8	2266.5		2265.1		2263.8	2268.4		2266.2				2266.0	1.6	4	2
97	(disaccharide)							2271.2	2272.0					2271.6	0.6	0	2
98		2501.6										2504.8		2503.2	2.3	1	1
99	(sterol)	2802.4	2799.8		2798.0		2801.5			2812.1	2814.8	2808.8		2805.4	6.5	4	3
100	(trisaccharide)				2910.2	2915.5	2916.3			2926.9		2930.1		2919.8	8.4	3	2
101	stigmastanol	3002.9	3004.6		3001.1	3005.5	3004.6				3017.0			3006.0	5.6	5	1
102	β-sitosterol				3004.6									3004.6	-	1	0
103	(sterol)				3055.8									3055.8	-	1	0
	Total # of Peaks Observed In Sample	27	33	23	38	30	35	50	27	43	29	41	24				

Appendix 3

GC-TOF Data For Synthesized C_5-Tetrols

GCT Data 1: GCT Probe Mass Spectrum of Synthesized C_5-Tetrols

GCT Data 2: Elemental Composition Report of *m/z* 105

^{1}H-NMR and ^{13}C-NMR Data For Synthesized C_5-Tetrols

NMR Data 1: ^{1}H and ^{13}C NMR Summary of Synthesized C_5-Tetrols

NMR Data 2: Theoretical ^{13}C Shifts of Synthesized C_5-Tetrols

NMR Data 3: ^{1}H NMR of Synthesized C_5-Tetrols in DMSO-d_6

NMR Data 4: ^{1}H NMR of Synthesized C_5-Tetrols in DMSO-d_6 (3.1-4.5 ppm)

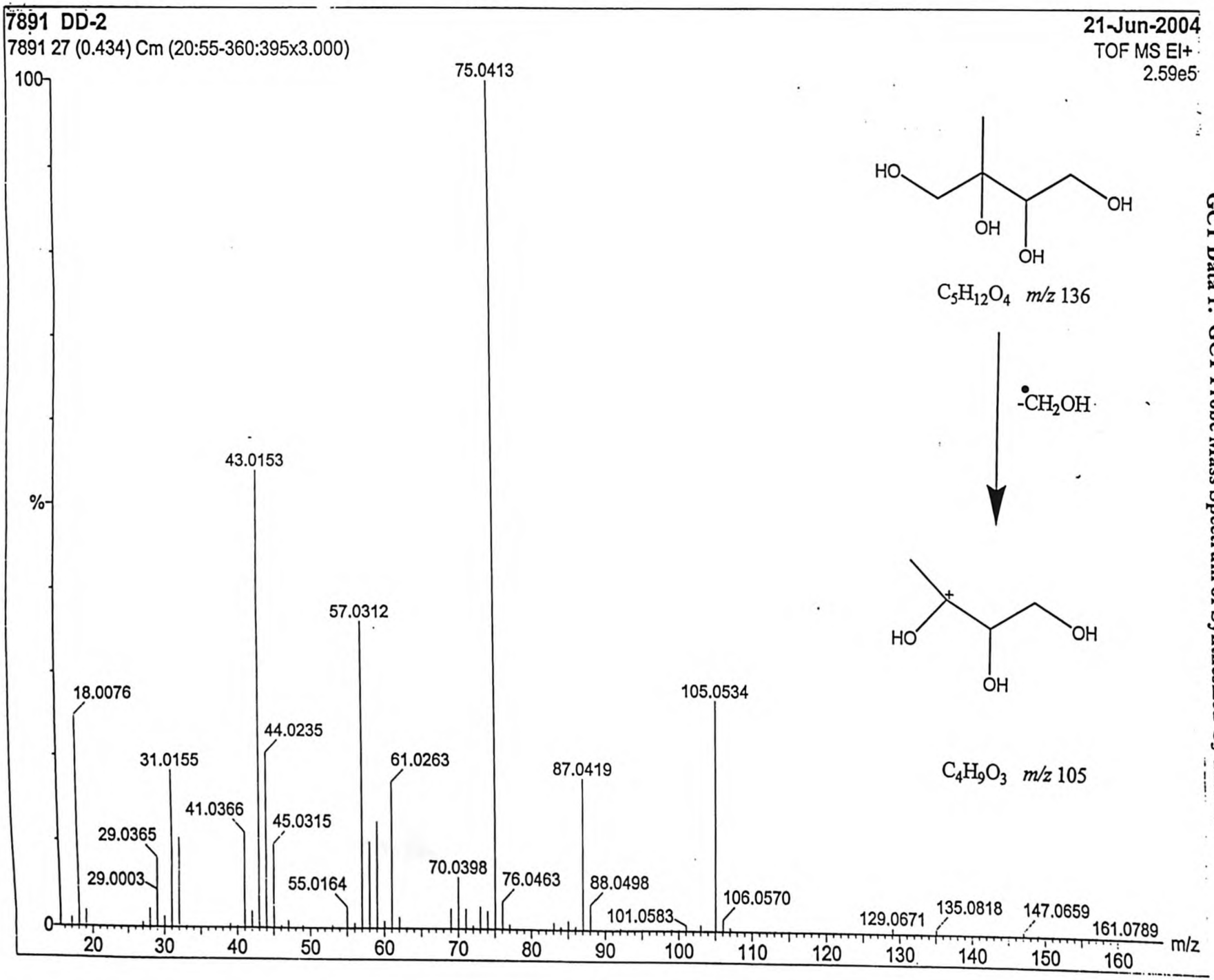
NMR Data 5: ^{1}H NMR of Synthesized C_5-Tetrols in DMSO-d_6 (0.70-1.35 ppm)

NMR Data 6: ^{1}H NMR of Synthesized C_5-Tetrols in DMSO-d_6 + D_2O

NMR Data 7: ^{13}C NMR of Synthesized C_5-Tetrols in DMSO-d_6

NMR Data 8: ^{13}C NMR of Synthesized C_5-Tetrols in DMSO-d_6 (61-77 ppm)

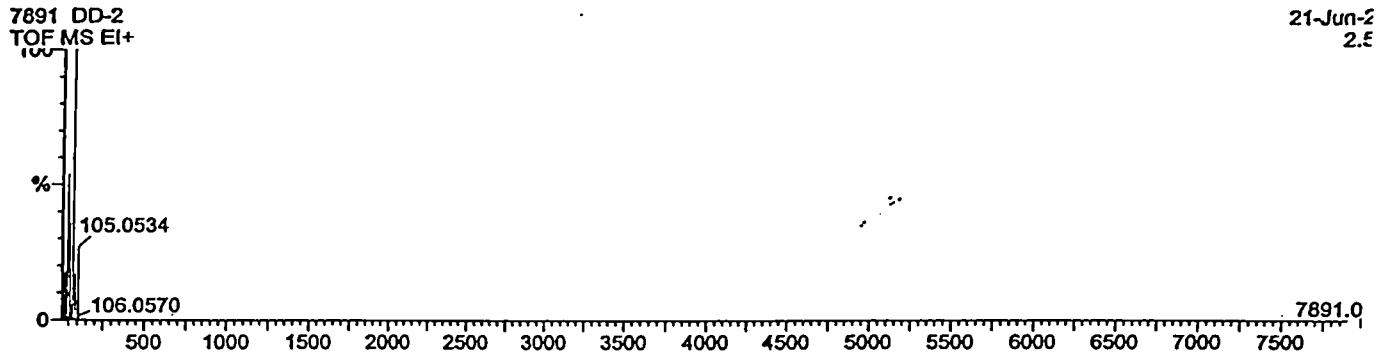
NMR Data 9: ^{13}C NMR of Synthesized C_5-Tetrols in DMSO-d_6 (17-25 ppm)



GCT Data 1: GCT Probe Mass Spectrum of Synthesized C_5-Tetrols

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

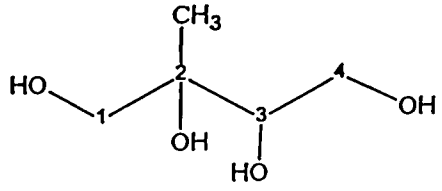
Monoisotopic Mass, Odd and Even Electron Ions
37 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)



Minimum:				-1.5		
Maximum:		10.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
105.0534	105.0538	-0.4	-3.9	1.0	2	C2 H7 N3 O2
	105.0552	-1.7	-16.6	0.5	1	C4 H9 O3 ←
	105.0578	-4.4	-42.2	5.0	4	C7 H7 N
	105.0453	8.1	77.6	5.5	3	C6 H5 N2

GCT Data 2: Elemental Composition Report of *m/z* 105

NMR Data 1: ^{1}H and ^{13}C NMR Summary of Synthesized C_5-Tetrols



TOP FRACTION:

TABLE 1. ^{1}H Chemical shifts for the high and low concentration components of the top fraction sample in DMSO-d_6.

PROTON	CHEMICAL SHIFT (ppm)	
	High	Low
1a	3.322 (3.222)[a]	3.283 (3.284)
1b	3.191 (3.191)	3.226 (3.228)
2-CH_3	0.995 (0.993)	0.937 (0.935)
3	3.36[b]	3.388 (3.388)
4a	3.539 (3.538)	3.596 (3.596)
4b	3.36[b]	3.36[b]

[a] The values in brackets represent the corresponding signals of the bottom fraction.
[b] Estimated chemical shifts owing to signal overlap.

TABLE 2. $^{1}H - {}^{1}H$ Coupling constants for the high and low concentration components of the top fraction sample in DMSO-d_6.

PROTONS	COUPLING CONSTANT (Hz)	
	High	Low
^{3}J		
4a,3	1.2 (1.2)[a]	3.3 (3.2)
4b,3	[b]	7.6 (7.6)
^{2}J		
1a,1b	-10.6 (-10.7)	-10.9 (-10.9)
4a,4b	-8.7 (-8.8)	-10.8 (-10.8)

[a] The values in brackets represent the corresponding signals of the bottom fraction.

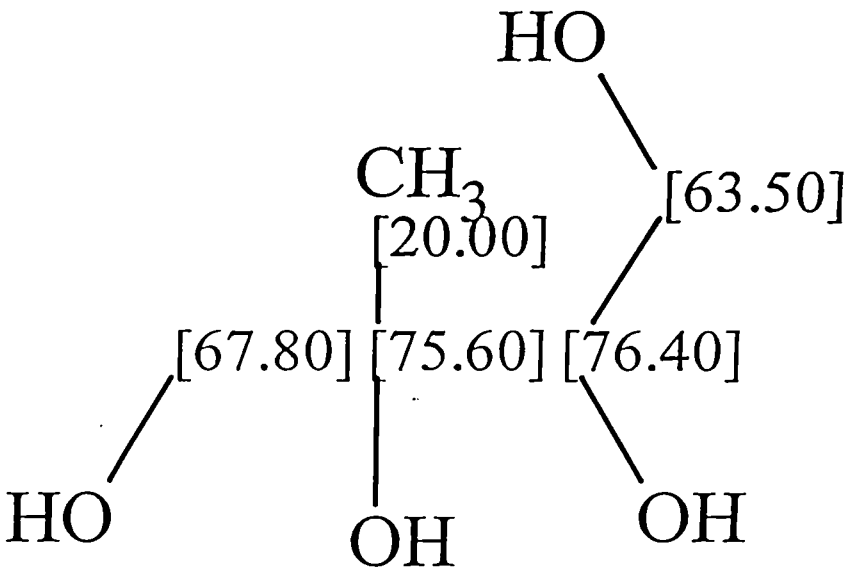
[b] Coupling constant not resolved owing to signal overlap.

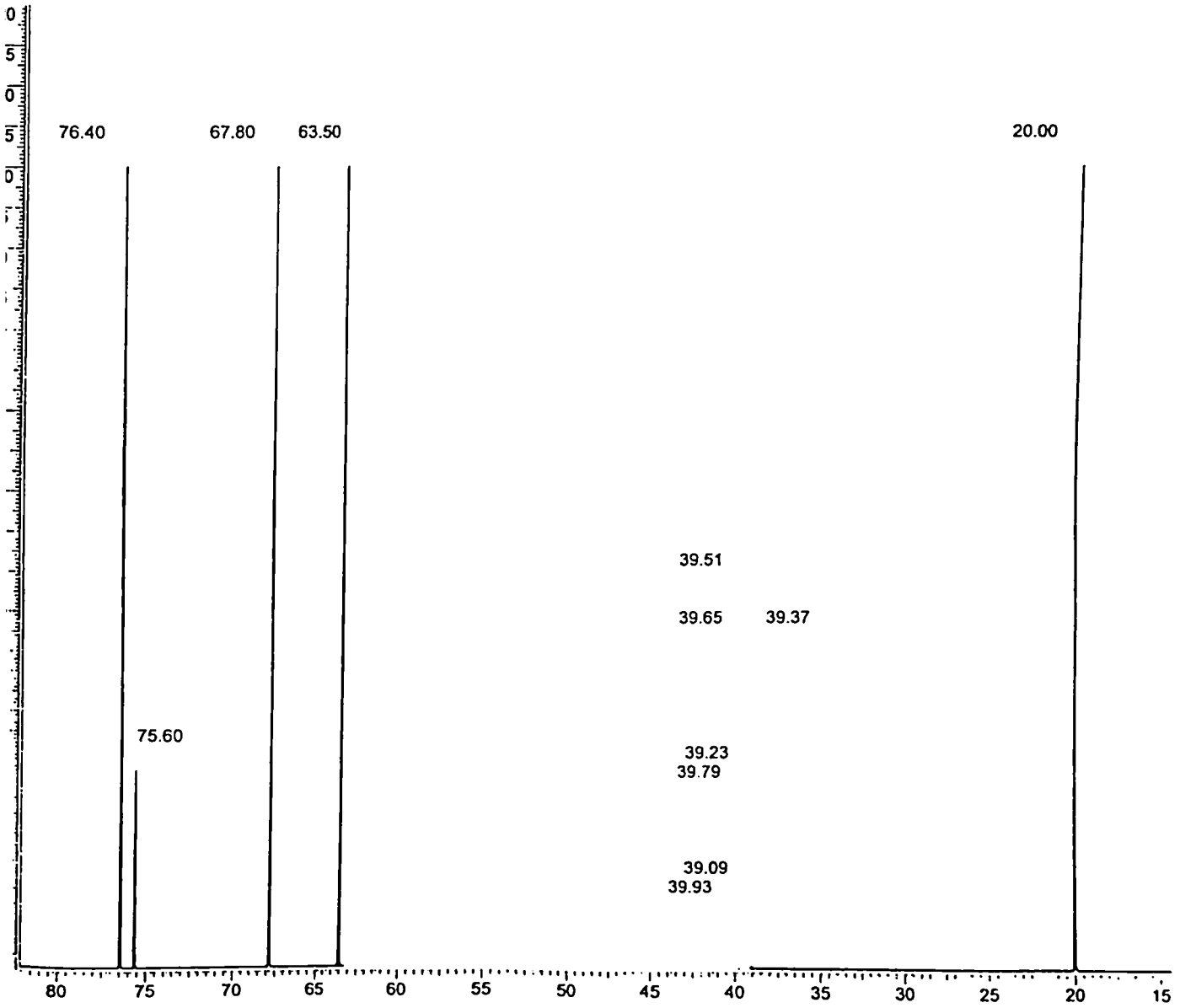
TABLE 3. ^{13}C Chemical shifts for the high and low concentration components of the top fraction sample in DMSO-d_6.

CARBON	CHEMICAL SHIFT (ppm)	
	High	Low
1	66.37 (66.39)[a]	67.27 (67.28)
2	73.28 (73.30[b])	73.28 (73.32[b])
2-CH_3	21.53 (21.56)	19.43 (19.44)
3	75.51 (75.52)	74.35 (74.36)
4	62.18 (62.19)	62.26 (62.28)

[a] The values in brackets represent the corresponding signals of the bottom fraction.
[b] Assignments may be reversed.

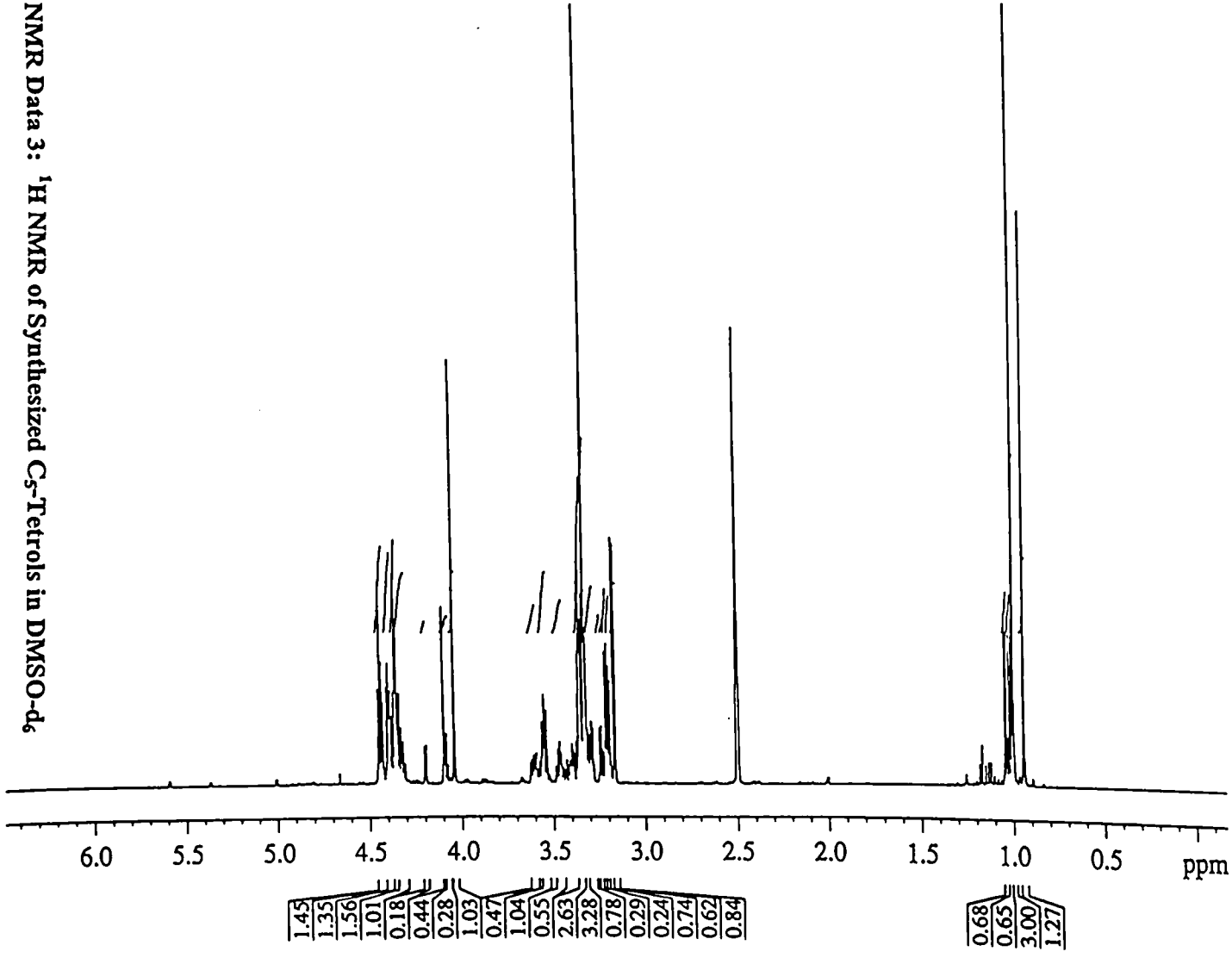
NMR Data 2: Theoretical ^{13}C Shifts of Synthesized C_5-Tetrols





Top Fraction
1H NMR in DMSO-d6 (6 July 2004)

NMR Data 3: ^{1}H NMR of Synthesized C_5-Tetrols in DMSO-d_6



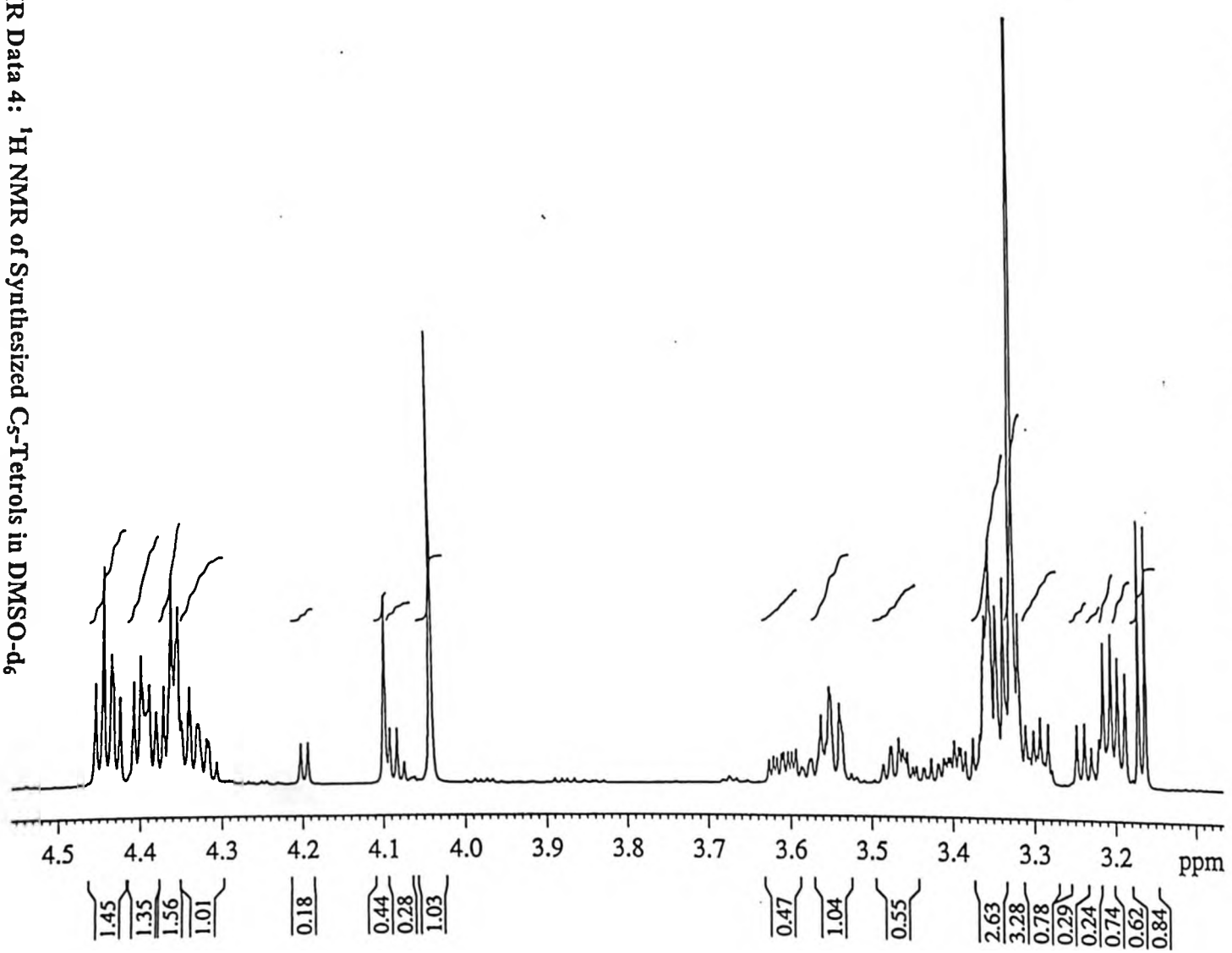
Current Data Parameters
NAME daviddam
EXPNO 1
PROCNO 1

F2 – Acquisition Parameters
Date_ 20040706
Time 14.52
INSTRUM av600
PROBHD 5 mm TBI 1H-13
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 4595.588 Hz
FIDRES 0.070123 Hz
AQ 7.1304755 sec
RG 90.5
DW 108.800 usec
DE 6.00 usec
TE 298.0 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 8.00 usec
PL1 -2.00 dB
SFO1 600.1317419 MHz

F2 – Processing parameters
SI 65536
SF 600.1300070 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

Top Fraction
1H NMR in DMSO–d6 (6 July 2004)



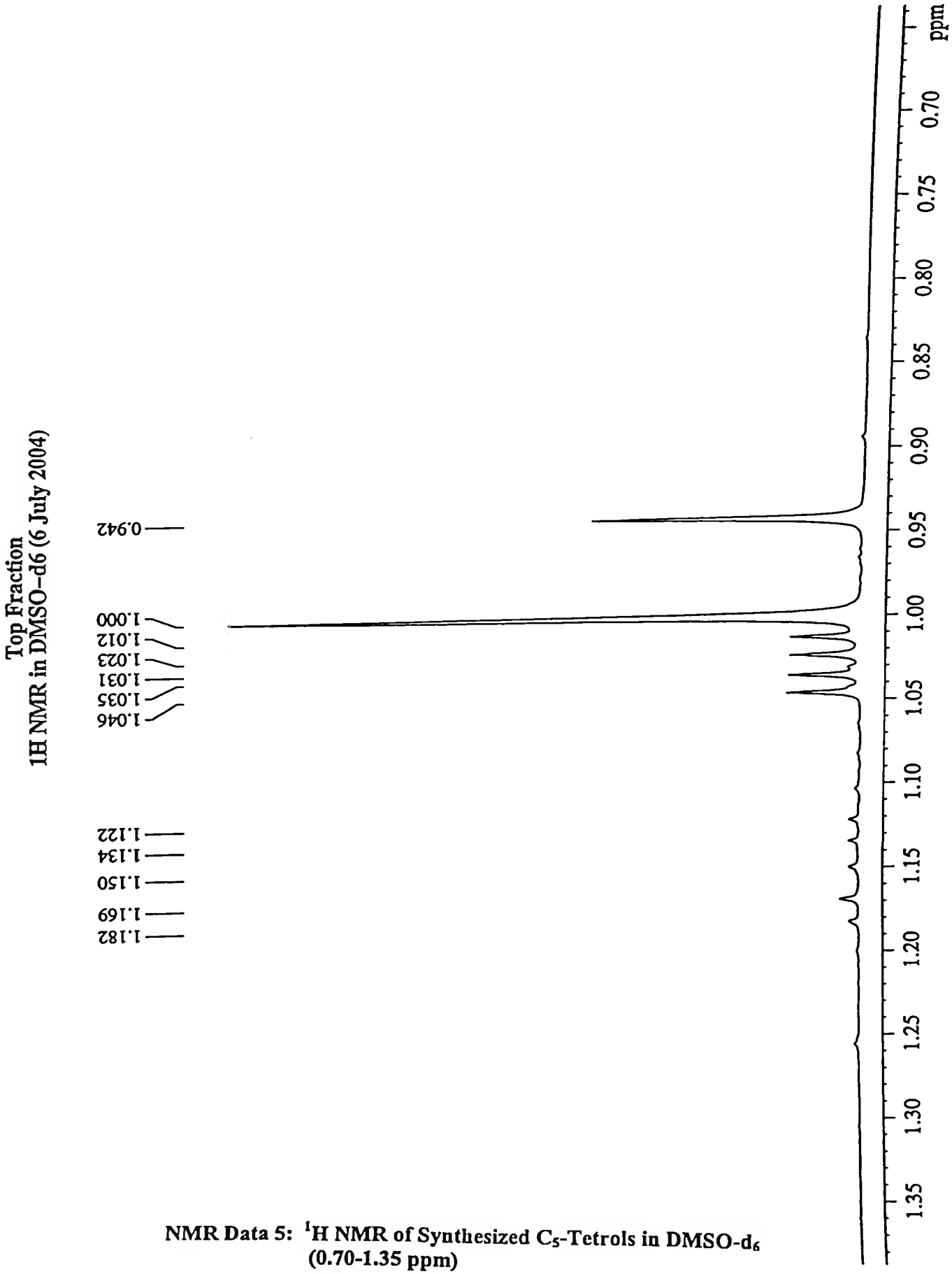
Current Data Parameters
NAME daviddam
EXPNO 1
PROCNO 1

F2 – Acquisition Parameters
Date_ 20040706
Time 14.52
INSTRUM av600
PROBHD 5 mm TBI 1H–13
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 4595.588 Hz
FIDRES 0.070123 Hz
AQ 7.1304755 sec
RG 90.5
DW 108.800 usec
DE 6.00 usec
TE 298.0 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 8.00 usec
PL1 –2.00 dB
SFO1 600.1317419 MHz

F2 – Processing parameters
SI 65536
SF 600.1300070 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

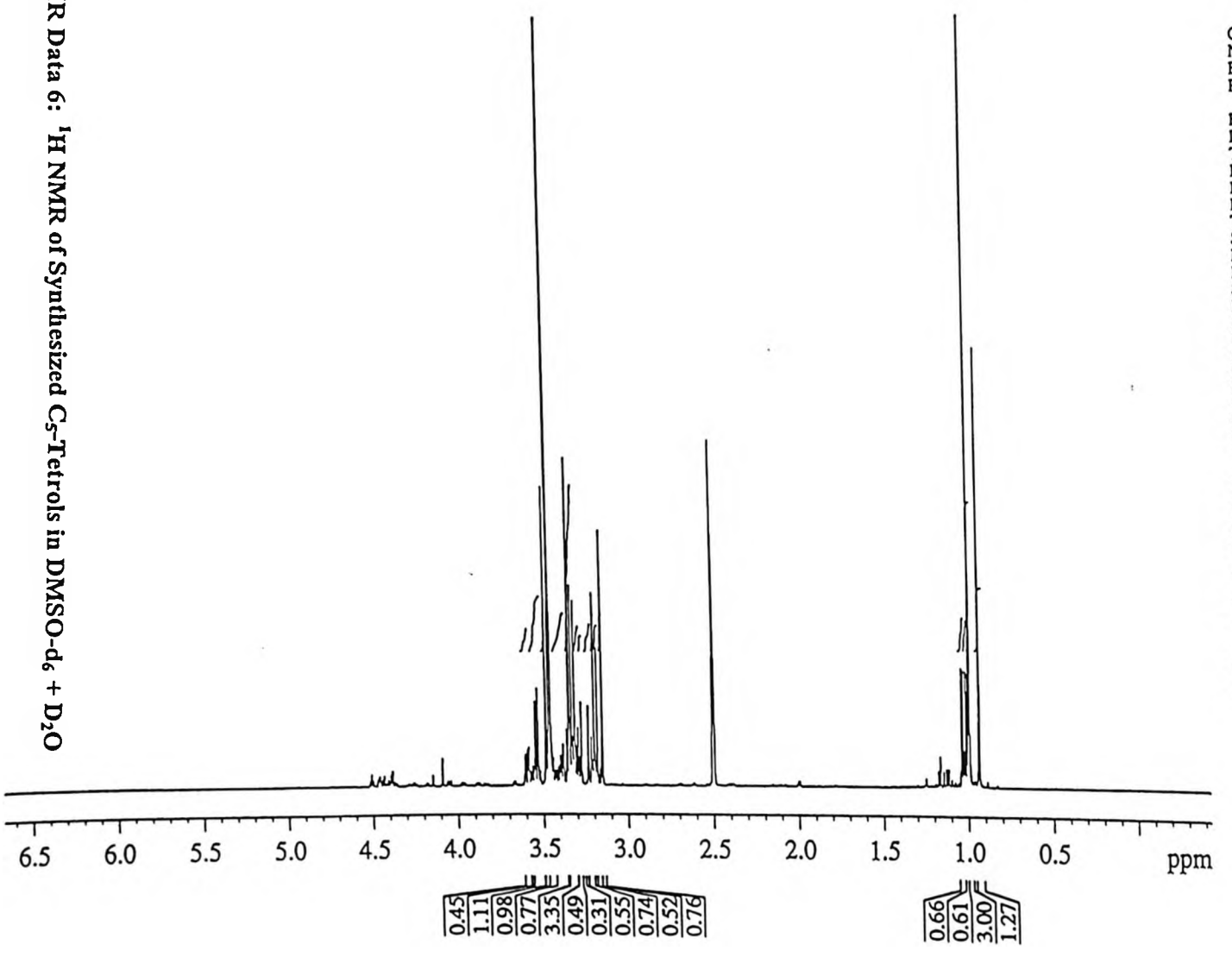
NMR Data 4: ^{1}H NMR of Synthesized C_5-Tetrols in DMSO-d_6 (3.1-4.5 ppm)



NMR Data 5: ^{1}H NMR of Synthesized C_5-Tetrols in DMSO-d_6 (0.70-1.35 ppm)

NMR Data 6: ^{1}H NMR of Synthesized C_5-Tetrols in DMSO-d_6 + D_2O

Top Fraction
1H NMR in DMSO–d6 + 1 drop D2O (6 July 2004)



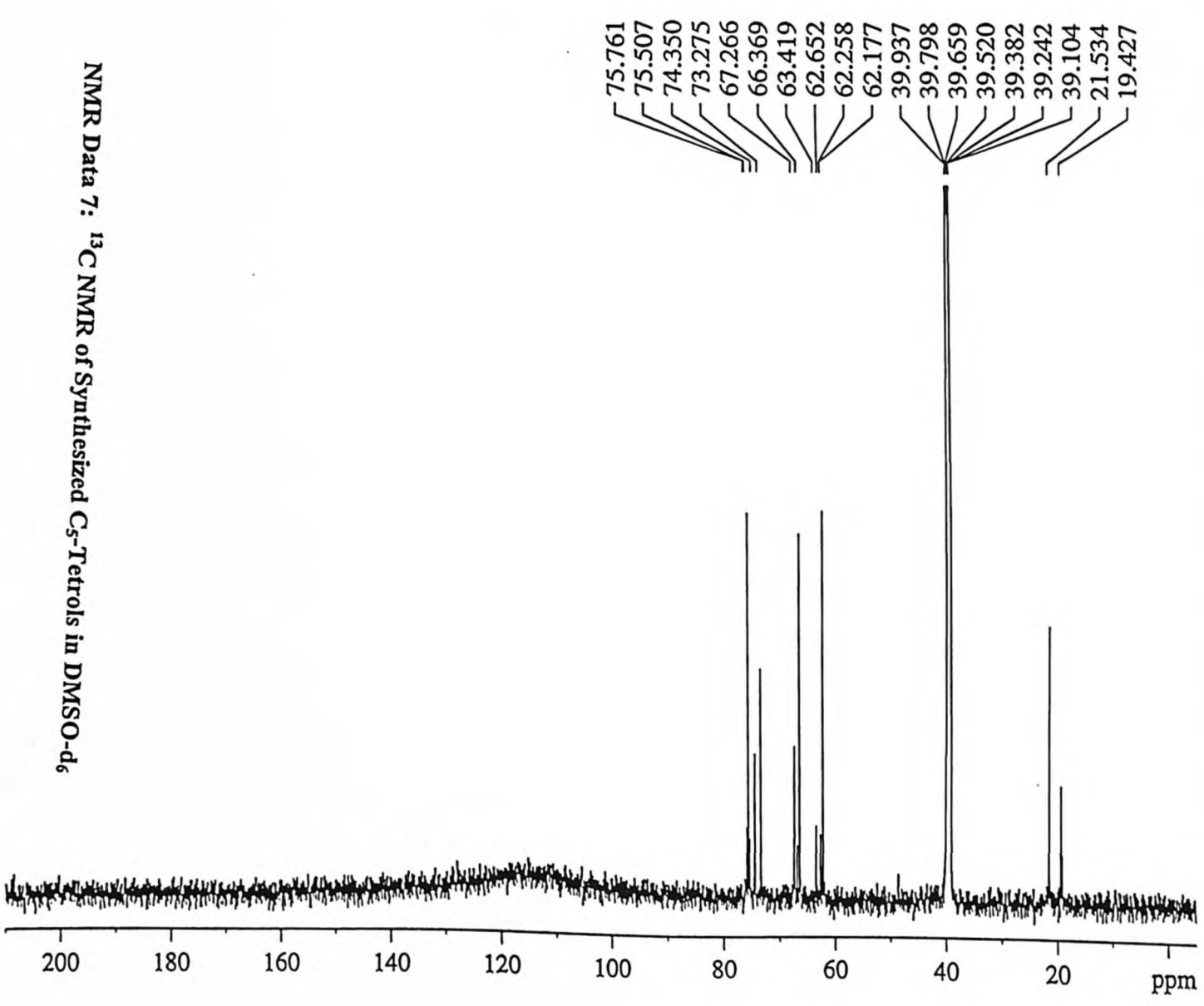
Current Data Parameters
NAME daviddam
EXPNO 5
PROCNO 1

F2 – Acquisition Parameters
Date_ 20040706
Time 16.20
INSTRUM av600
PROBHD 5 mm TBI 1H–13
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 4595.588 Hz
FIDRES 0.070123 Hz
AQ 7.1304755 sec
RG 90.5
DW 108.800 usec
DE 6.00 usec
TE 298.0 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 8.00 usec
PL1 –2.00 dB
SFO1 600.1317419 MHz

F2 – Processing parameters
SI 65536
SF 600.1300070 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

13C NMR in DMSO-d6 (6 July 2004)



NMR Data 7: ^{13}C NMR of Synthesized C_5-Tetrols in DMSO-d_6

BRUKER

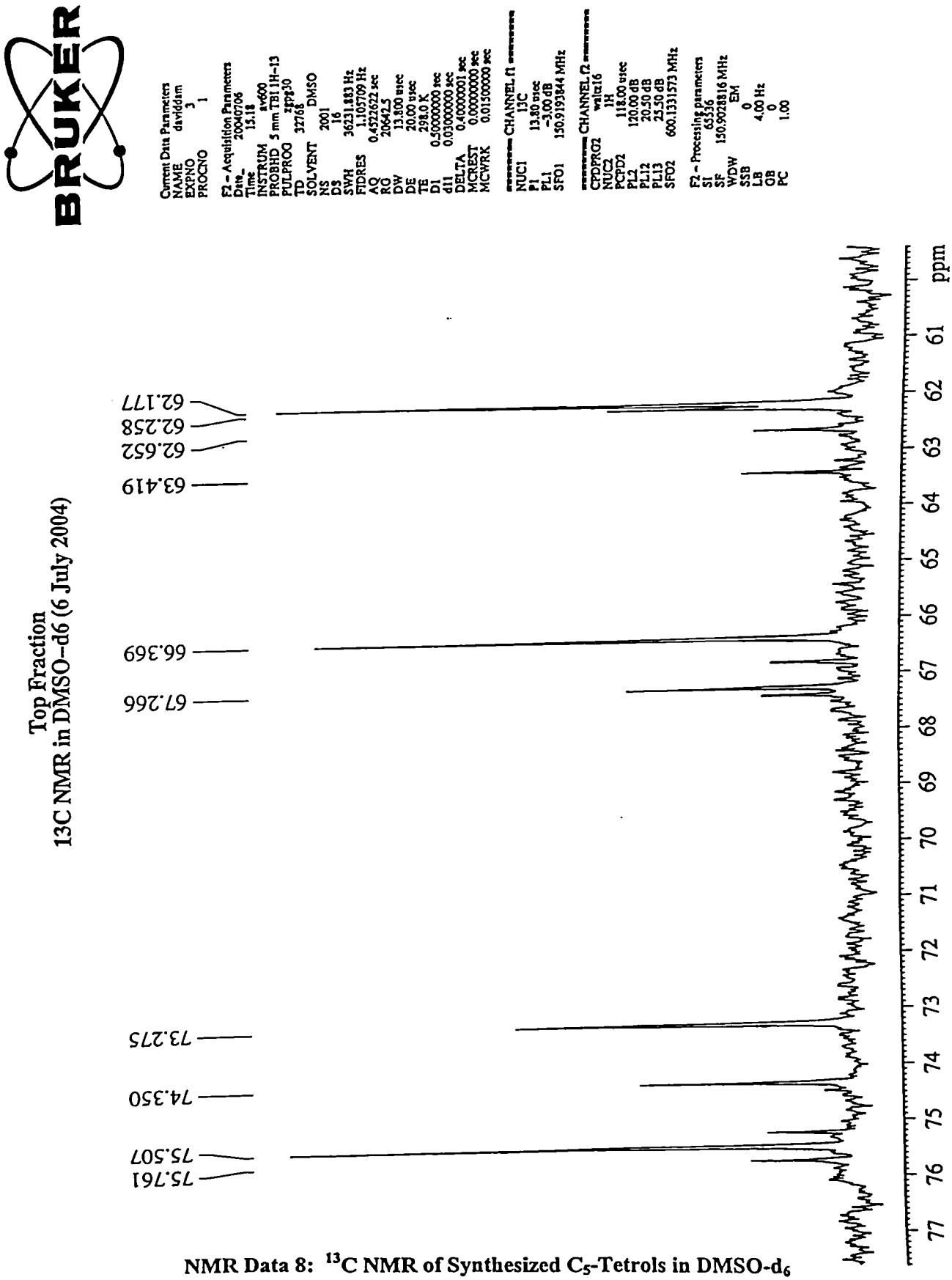
Current Data Parameters
NAME daviddam
EXPNO 3
PROCNO 1

F2 – Acquisition Parameters
Date_ 20040706
Time 15.18
INSTRUM av600
PROBHD 5 mm TBI 1H–13
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 2001
DS 16
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.4522622 sec
RG 20642.5
DW 13.800 usec
DE 20.00 usec
TE 298.0 K
D1 0.50000000 sec
d11 0.03000000 sec
DELTA 0.40000001 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 13.80 usec
PL1 -3.00 dB
SFO1 150.9193844 MHz

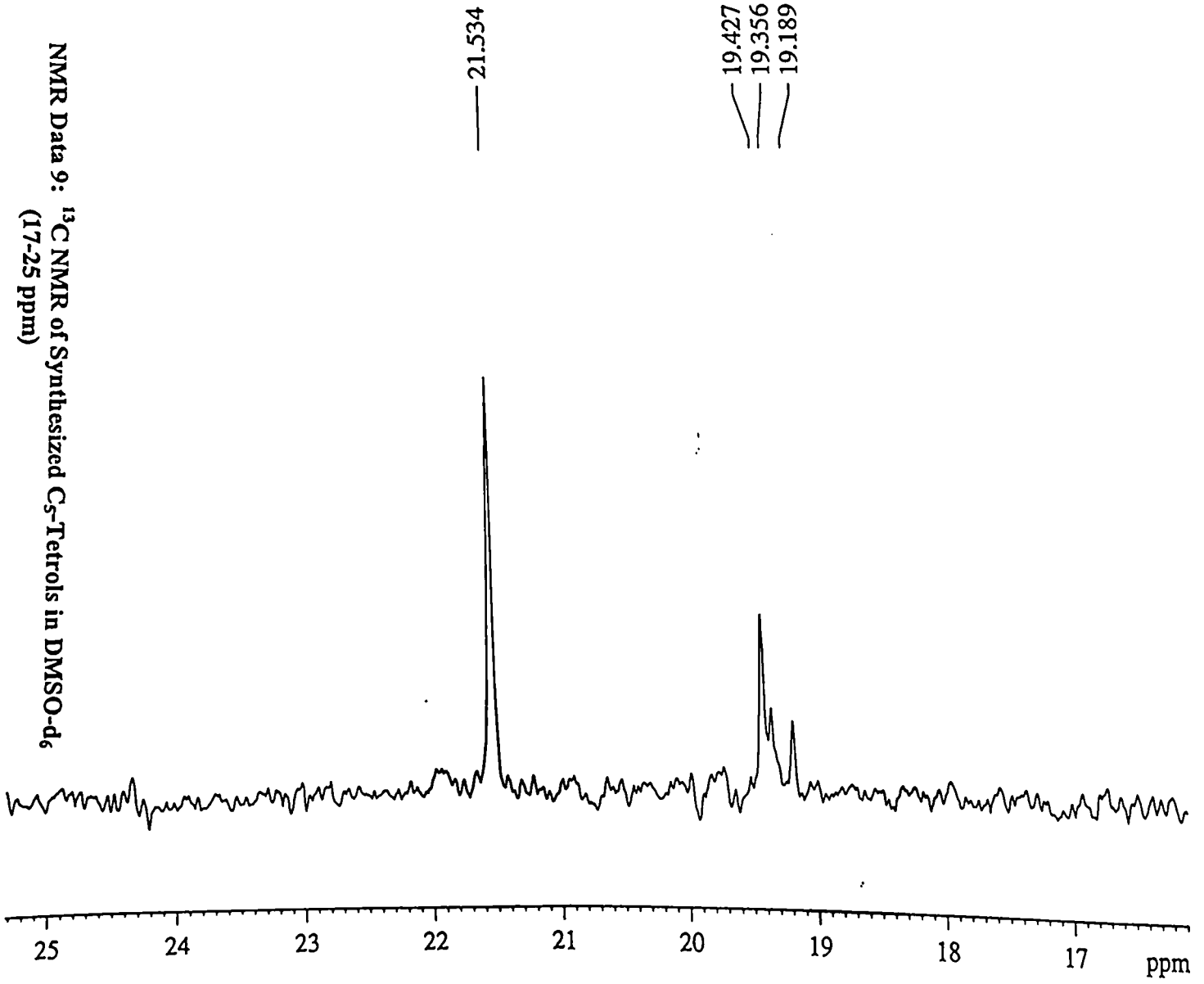
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 118.00 usec
PL2 120.00 dB
PL12 20.50 dB
PL13 25.50 dB
SFO2 600.1331573 MHz

F2 – Processing parameters
SI 65536
SF 150.9028816 MHz
WDW EM
SSB 0
LB 4.00 Hz
GB 0
PC 1.00



NMR Data 8: ^{13}C NMR of Synthesized C_5-Tetrols in DMSO-d_6 (61-77 ppm)

Top Fraction
13C NMR in DMSO–d6 (6 July 2004)



NMR Data 9: ^{13}C NMR of Synthesized C_5-Tetrols in DMSO-d_6 (17-25 ppm)

Current Data Parameters
NAME daviddam
EXPNO 3
PROCNO 1

F2 – Acquisition Parameters
Date_ 20040706
Time 15.18
INSTRUM av600
PROBHD 5 mm TBI 1H–13
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 2001
DS 16
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.4522622 sec
RG 20642.5
DW 13.800 usec
DE 20.00 usec
TE 298.0 K
D1 0.50000000 sec
d11 0.03000000 sec
DELTA 0.40000001 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 13.80 usec
PL1 –3.00 dB
SFO1 150.9193844 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 118.00 usec
PL2 120.00 dB
PL12 20.50 dB
PL13 25.50 dB
SFO2 600.1331573 MHz

F2 – Processing parameters
SI 65536
SF 150.9028816 MHz
WDW EM
SSB 0
LB 4.00 Hz
GB 0
PC 1.00

Appendix 4

Concentrations of analytes found in the methanol extracts and dichloromethane extracts of window films sampled at various sites. Data provided by R. Chen[1], but not included in her thesis.

Nomenclature:

1) Aliphatic monocarboxylic acids (fatty acids)

11E: undecanoic acid
12E: dodecanoic acid, lauric acid
13E: tridecanoic acid
14E: tetradecanoic acid
15E: pentadecanoic acid
16E: hexadecanoic acid, palmitic acid
17E: heptadecanoic acid
18E: octadecanoic acid, steric acid
19E: nonadecanoic acid
20E: eicosanoic acid
21E: henelcosanoic acid
22E: docosanoic acid
23E: tricosanoic acid
24E: tetracosanoic acid
25E: petacosanoic acid
26E: hexacosanoic acid
27E: heptacosanoic acid
28E: octacosanoic acid
29E: nonacosanoic acid
30E: decacosanoic acid
31E: undecacosanoic acid

2) Aliphatic dicarboxylic acids

2DE: oxalic acid, ethanedioic acid
3DE: malonic acid, propanedioic acid.
4DE: succinic acid, butanedioic acid
5DE: glutaric acid, petanedioic acid
6DE: adipic acid, hexanedioic acid
7DE: pimelic acid, heptanedioic acid
8DE: suberic acid, octanedioic acid
9DE: azelaic acid, nonanedioic acid.
10DE: sebacic acid, decanedioic acid
11DE: undecanedioic acid
12DE: dodecanedioic acid
13DE: tridecanedioic acid
14DE: tetradecanedioic acid

3) Aromatic acids

ph: phthalic acid
tph: terephthalic acid
iph: isophthalic acid
c-ph: 4-methyl phthalic acid
124BE: 1,2,4- benzenetricarboxylic acid
123BE: 1,2,3-benzenetricarboxylic acid
135BE: 1,3,5-benzenetricarboxylic acid
1245BE: 1,2,4,5-benzenebutacarboxylic acid
12NE: 2,3-naphthalene dicarboxylic acid

4) Resin acids

PE: pimaric acid
SPE: sandaracopimaric acid
IPE: isopimaric acid
DHE: dihydroxy abietic acid
ODE: 7-oxo-dehydroabietic acid

Egbert Indoor (EBI)
MR 22/01

			Methanol extract				DCM extract				Total	Correction of blanks		Correction with 0.5DL				
name	Ion	DL	E Mass in sample (ng)	A Mass in sample (ng)	Vol correction *	Transfer to ng/m² **	E Mass in sample (ng/450ul)	A Mass in sample (ng/450ul)	Vol correction a	Transfer to ng/m² **	Total (ng/m²)	Total mass in ave FB (ng)	Corrected total (ng/m2)	Corrected total (ng/m2)		Mw		Mw
11E	74	0.10	61.7	57.39	114.8	10.1	0.05	0.05	1.03	0.09	10.17	1.13	9.91	10.07	11E	200	11a	186
12E	74	0.10	786.6	716.47	1432.9	125.8	75.55	70.60	1569.00	137.75	263.56	385.27	175.61	229.73	12E	214	12a	200
13E	74	0.10	56.8	53.34	106.7	9.4	15.88	14.91	331.28	29.09	38.45	1.14	38.19	38.35	13E	228	13a	214
14E	74	0.10	488.9	460.63	921.3	80.9	221.15	208.36	4630.12	406.51	487.39	262.93	427.37	464.31	14E	242	14a	228
15E	74	0.10	331.6	313.51	627.0	55.0	130.23	123.11	2735.81	240.19	295.24	122.10	267.37	284.52	15E	256	15a	242
16E	74	0.15	3941.8	3737.39	7474.8	656.3	2235.18	2119.28	47095.19	4134.78	4791.04	4999.42	3649.82	4352.11	16E	270	16a	256
17E	74	0.10	210.2	199.85	399.7	35.1	139.47	132.59	2946.46	258.69	293.78	383.78	210.74	261.84	17E	284	17a	270
18E	74	0.10	1871.3	1783.43	3566.9	313.2	1222.53	1165.09	25890.92	2273.13	2586.28	3467.77	1790.13	2280.07	18E	298	18a	284
19E	74	0.10	118.3	112.96	225.9	19.8	74.06	70.73	1571.85	138.00	157.84	269.56	91.74	132.42	19E	312	19a	298
20E	74	0.10	1101.5	1054.18	2108.4	185.1	705.07	674.79	14995.27	1316.53	1501.63	3939.69	602.32	1155.74	20E	326	20a	312
21E	74	0.10	453.6	434.92	869.8	76.4	316.95	303.90	6753.28	592.91	669.28	1721.03	276.42	518.18	21E	340	21a	326
22E	74	0.15	1866.4	1792.59	3585.2	314.8	1409.40	1353.67	30081.48	2641.04	2955.81	7897.89	1196.61	2279.96	22E	354	22a	340
23E	74	0.10	895.9	861.80	1723.6	151.3	726.85	701.12	15580.40	1367.90	1519.23	3186.70	791.80	1239.45	23E	368	23a	354
24E	74	0.15	2418.6	2329.95	4659.9	409.1	2179.27	2099.40	46653.41	4096.00	4505.12	8738.25	2510.44	3737.93	24E	382	24a	368
25E	74	0.15	403.3	389.09	778.2	68.3	374.68	361.44	8031.95	705.18	773.50	1100.18	522.36	676.90	25E	396	25a	382
26E	74	0.15	992.5	958.60	1917.2	168.3	466.80	452.79	10062.09	883.41	1051.74	3581.97	234.06	737.25	26E	410	26a	396
27E	74	0.15	32.3	31.20	62.4	5.5	0.06	0.07	1.61	0.14	5.62	17.91	1.53	4.05	27E	424	27a	410
28E	74	0.15	219.5	212.49	425.0	37.3	152.69	147.81	3284.66	288.38	325.69	764.92	151.09	256.54	28E	438	28a	424
29E	74	0.25	0.13	0.12	0.2	0.02	0.13	0.12	2.69	0.24	0.26	2.93	-0.41	0.13	29E	452	29a	438
30E	74	0.25	0.13	0.12	0.2	0.02	0.13	0.12	2.69	0.24	0.26	2.94	-0.41	0.13	30E	466	30a	452
31E	74	0.25	0.13	0.12	0.2	0.02	0.13	0.12	2.70	0.24	0.26	2.94	-0.41	0.13	31E	480	31a	466
TOTAL			16231.3	15500.1	31000.3	2721.7				19510.44	22232.15	40670.44	12948.29	18661.81				
6DE	101	0.27	1288.4	1061.10	2162.2	189.8	0.13	0.11	2.51	0.22	190.05	78.37	172.16	183.17	6da	174	6da	146
7DE	115	0.30	721.7	614.16	1228.4	107.8	0.15	0.13	2.82	0.25	108.09	3.07	107.39	107.82	7da	188	7da	160
8DE	129	0.25	1655.2	1425.74	2851.5	250.3	106.96	92.13	2047.35	179.75	430.10	2.62	429.50	429.87	8da	202	8da	174
9DE	185	0.39	6066.6	5280.22	10560.4	927.2	390.57	339.94	7554.18	663.23	1590.40	138.64	1558.75	1578.23	9da	216	9da	188
10DE	199	0.31	152.2	133.71	267.4	23.5	24.89	21.86	485.82	42.65	66.13	3.30	65.38	65.84	10da	230	10da	202
11DE	213	0.44	161.8	143.23	286.5	25.2	0.22	0.19	4.30	0.38	25.53	4.69	24.46	25.12	11da	244	11da	216
12DE	227	0.57	209.8	187.04	374.1	32.8	0.29	0.26	5.67	0.50	33.34	6.18	31.93	32.80	12da	258	12da	230
13DE	241	0.49	96.6	86.64	173.3	15.2	0.24	0.22	4.84	0.42	15.64	5.27	14.43	15.17	13da	272	13da	244
14DE	255	0.97	106.8	96.14	196.3	17.2	0.49	0.44	9.76	0.86	18.09	10.64	15.66	17.16	14da	286	14da	258
TOTAL			10461.1	9050.0	18100.0	1589.1				888.26	2477.37	252.78	2419.67	2455.18				
tph	163	0.10	0.05	0.04	0.09	0.01	0.05	0.04	0.95	0.08	0.09	1.04	-0.15	0.05	tph	194	corre.acid	166
ph	163	0.10	3333.2	2852.09	5704.19	500.8	14.82	12.68	281.80	24.74	525.55	45.15	515.24	521.58	ph	194		166
iph	163	0.10	85.6	73.20	146.41	12.9	0.05	0.04	0.95	0.08	12.94	1.04	12.70	12.85	iph	194		166
o-ph	177	0.05	52.4	45.34	90.67	8.0	0.03	0.02	0.48	0.04	8.00	4.40	7.00	7.62	o-ph	208		180
124BE	221	0.05	138.6	115.50	231.00	20.3	0.03	0.02	0.46	0.04	20.32	1.01	20.09	20.23	124be	252		210
123BE	221	0.05	59.4	49.47	98.93	8.7	0.03	0.02	0.46	0.04	8.73	9.03	6.66	7.93	123be	252		210
135BE	221	0.05	0.03	0.02	0.04	0.00	0.03	0.02	0.46	0.04	0.04	1.05	-0.19	0.03	135be	252		210
1245BE	279	0.02	3.3	2.66	5.36	0.5	0.01	0.01	0.18	0.02	0.49	0.20	0.44	0.47	1245be	310		254
12NE	213	0.05	0.03	0.02	0.04	0.00	0.03	0.02	0.49	0.04	0.05	0.54	-0.06	0.03	12ne	244		216
TOTAL			3672.4	3138.37	6276.7	551.1				25.13	576.21	63.45	561.72	570.76				
PE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.02	0.23	-0.03	0.01	PE	316	corre.acid	302
SPE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.02	0.23	-0.03	0.01	SPE	316		302
IPE	241	0.08	0.04	0.04	0.08	0.01	0.04	0.04	0.85	0.07	0.08	0.93	-0.13	0.04	IPE	316		302
DHE	239	0.02	30.3	26.94	57.88	5.1	15.69	14.99	333.07	29.24	34.32	128.06	5.09	23.06	DHE	314		300
ODE	253	0.08	33.0	31.57	63.13	5.5	10.74	10.28	228.54	20.06	25.61	18.59	21.36	23.96	ODE	328		314
TOTAL			63.3	60.6	121.1	10.6				49.42	60.05	148.04	26.28	47.12				
TOTAL ACIDS						4872.5				20473.2	25345.8	41134.7	15955.8	21734.9				

* Total volume is 10.0 mL Analysed volume is 5.0 ml
** Sampling area is 11.39 m²
a: Total volume is 10.0 mL Analysed volume is 1.35 ml
Gravimetric W (mg m⁻³) 17.1
Kimwipes: 26

% corr./noncorr.
86

Egbert Outdoor (EBO)
MR 15/01

			Methanol extract				DCM extract				Total	Correction of blanks		Correction with 0.5 DL				
name	Ion	DL	E Mass in sample (ng)	A Mass in sample (ng)	Vol correction *	Transfer to ng/m³ **	E Mass in sample (ng/450uL)	A Mass in sample (ng/450uL)	Vol correction *	Transfer to ng/m³ **	Total (ng/m³)	Total mass in ave FB (ng)	Corrected total (ng/m³)	Corrected total (ng/m³)		Mw		Mw
11E	74	0.10	0.05	0.05	0.09	0.01	0.05	0.05	1.03	0.09	0.09	1.13	-0.13	0.05	11E	200	11a	186
12E	74	0.10	166.6	157.54	315.07	26.1	22.56	21.06	468.49	38.85	64.97	385.27	-11.70	0.05	12E	214	12a	200
13E	74	0.10	0.05	0.05	0.09	0.01	0.05	0.05	1.04	0.09	0.09	1.14	-0.13	0.05	13E	228	13a	214
14E	74	0.10	128.8	121.33	242.65	20.1	60.35	56.85	1263.43	104.78	124.88	262.93	72.56	72.56	14E	242	14a	228
15E	74	0.10	64.7	61.20	122.40	10.1	48.87	46.19	1026.56	85.12	95.27	122.10	70.97	70.97	15E	256	15a	242
16E	74	0.15	3061.4	2902.64	5805.28	481.4	1439.75	1365.09	30335.40	2515.37	2996.74	4999.42	2001.83	2001.83	16E	270	16a	256
17E	74	0.10	141.2	134.21	268.41	22.3	59.23	56.31	1251.44	103.77	126.02	363.78	53.63	53.63	17E	284	17a	270
18E	74	0.10	1678.4	1597.67	3195.34	265.0	527.94	503.13	11180.74	927.09	1192.05	3457.77	497.96	497.96	18E	298	18a	284
19E	74	0.10	189.2	180.82	361.64	30.0	37.14	35.47	788.25	65.36	95.35	289.56	37.72	37.72	19E	312	19a	298
20E	74	0.10	2254.3	2157.47	4314.95	357.8	337.49	322.99	7177.63	595.16	952.95	3939.69	168.93	168.93	20E	326	20a	312
21E	74	0.10	968.0	928.11	1856.22	153.9	136.50	130.88	2908.42	241.16	395.06	1721.03	52.58	52.58	21E	340	21a	326
22E	74	0.15	4988.3	4791.04	9582.07	794.5	680.80	653.67	14530.52	1204.85	1999.39	7897.89	467.47	467.47	22E	354	22a	340
23E	74	0.10	2316.7	2228.61	4457.22	369.6	284.81	273.97	6088.23	504.83	874.41	3186.70	240.25	240.25	23E	368	23a	354
24E	74	0.15	6030.9	5809.91	11619.83	963.5	974.68	938.96	20865.68	1730.18	2693.66	8738.25	954.70	954.70	24E	382	24a	368
25E	74	0.15	1018.0	980.04	1960.09	162.5	193.69	186.84	4151.97	344.28	506.80	1100.18	287.66	287.66	25E	396	25a	382
26E	74	0.15	2693.7	2592.03	5184.06	429.9	1037.92	1002.48	22277.23	1847.20	2277.06	3581.97	1564.22	1564.22	26E	410	26a	396
27E	74	0.15	159.6	154.35	308.70	25.6	94.96	91.84	2040.66	169.23	194.82	17.91	191.26	191.26	27E	424	27a	410
28E	74	0.15	822.2	795.89	1591.77	132.0	959.06	926.41	20631.33	1710.72	1842.71	784.92	1690.49	1690.49	28E	438	28a	424
29E	74	0.25	0.13	0.12	0.24	0.02	33.39	32.25	718.94	59.61	59.63	2.93	59.05	59.05	29E	452	29a	438
30E	74	0.25	0.13	0.12	0.24	0.02	87.35	84.73	1882.89	156.13	156.15	2.94	153.56	153.56	30E	466	30a	452
31E	74	0.25	0.13	0.12	0.24	0.02	0.13	0.12	2.70	0.22	0.24	2.94	-0.34	0.13	31E	480	31a	466
TOTAL			26670.5	25593.31	51186.6	4244.3	7016.70	6731.88		12404.04	16648.37	40670.44	8554.75	8567.34				
6DE	101	0.27	144.3	121.09	242.2	20.1	0.13	0.11	2.51	0.21	20.29	78.37	4.69	4.69	6de	174	6da	148
7DE	115	0.30	110.8	100.96	202.0	16.7	29.42	25.04	556.34	46.13	62.88	3.07	62.27	62.27	7de	188	7da	160
8DE	129	0.25	0.13	0.11	0.2	0.02	0.13	0.11	2.40	0.20	0.22	2.62	-0.30	0.13	8de	202	8da	174
9DE	185	0.39	370.8	322.52	645.0	53.5	42.57	37.05	823.42	68.28	121.76	136.64	94.17	94.17	9de	218	9da	188
10DE	199	0.31	0.16	0.14	0.3	0.02	0.16	0.14	3.03	0.25	0.27	3.30	-0.38	0.16	10de	230	10da	202
11DE	213	0.44	0.22	0.19	0.4	0.03	0.22	0.19	4.30	0.36	0.39	4.69	-0.54	0.22	11de	244	11da	216
12DE	227	0.57	0.29	0.26	0.5	0.04	0.29	0.26	5.67	0.47	0.51	6.18	-0.72	0.29	12de	258	12da	230
13DE	241	0.49	0.24	0.22	0.4	0.04	0.24	0.22	4.84	0.40	0.44	5.27	-0.61	0.24	13de	272	13da	244
14DE	255	0.97	0.49	0.44	0.9	0.07	0.49	0.44	9.76	0.81	0.88	10.64	-1.24	0.49	14de	286	14da	258
TOTAL			635.0	545.84	1091.9	90.5				117.10	207.64	252.78	157.34	162.65				
tph	183	0.10	0.05	0.04	0.09	0.01	0.05	0.04	0.95	0.08	0.09	1.04	-0.12	0.05	tph	194	comr.acid	166
ph	183	0.10	128.4	109.83	219.66	18.2	3.46	2.96	65.80	5.46	23.67	45.15	14.68	14.68	ph	194		166
lph	183	0.10	0.05	0.04	0.09	0.01	0.05	0.04	0.95	0.08	0.09	1.04	-0.12	0.05	lph	194		166
o-ph	177	0.05	12.9	11.19	22.38	1.9	0.03	0.02	0.48	0.04	1.90	4.40	1.02	1.02	o-ph	208		180
124BE	221	0.05	2.9	2.45	4.90	0.4	0.03	0.02	0.48	0.04	0.44	1.01	0.24	0.24	124be	252		210
123BE	221	0.05	17.8	14.81	29.62	2.5	0.03	0.02	0.48	0.04	2.49	9.03	0.70	0.70	123be	252		210
135BE	221	0.05	1.6	1.36	2.73	0.2	0.03	0.02	0.48	0.04	0.26	1.05	0.06	0.06	135be	252		210
1245BE	279	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.18	0.02	0.02	0.20	-0.02	0.01	1245be	310		254
12ME	213	0.05	0.03	0.02	0.04	0.00	0.03	0.02	0.49	0.04	0.04	0.54	-0.06	0.03	12me	244		216
TOTAL			163.8	139.78	279.5	23.2				5.82	29.00	63.45	16.38	16.84				
PE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.02	0.23	-0.03	0.01	PE	316	comr.acid	302
SPE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.02	0.23	-0.03	0.01	SPE	316		302
IPE	241	0.06	0.04	0.04	0.08	0.01	0.04	0.04	0.85	0.07	0.08	0.93	-0.11	0.04	IPE	316		302
DHE	239	0.02	20.9	19.93	39.86	3.3	22.70	21.69	461.96	39.96	43.27	128.06	17.78	32.63	DHE	314		300
ODE	253	0.06	0.03	0.03	0.06	0.00	11.77	11.27	250.50	20.77	20.78	18.59	17.06	19.23	ODE	328		314
TOTAL			20.9	20.01	40.0	3.3				60.84	64.16	148.04	34.70	51.84				
TOTAL ACIDS						4361.4				12587.8	16949.2	41134.7	8763.2	8798.8				

* Total volume	10.0 mL	Analysed volume	8.0 ml		% commoncorr
** Sampling area	12.08 m²				52
a: Total volume	10.0 mL	Analysed volume	1.56 ml		
Gravimetric W (mg m⁻³)	93.1				
# Kimwipes:	24				

Residential indoor (RSI)
MR 15/01

			Methanol extract				DCM extract				Total	Correction of blanks		Correction with 0.5DL				
name	Ion	DL	E Mass in sample (ng)	A Mass in sample (ng)	Vol correction *	Transfer to ng/m² **	E Mass in sample (ng/450uL)	A Mass in sample (ng/450uL)	Vol correction *	Transfer to ng/m² **	Total (ng/m²)	Total mass in sve FB (ng)	Corrected total (ng/m²)	Corrected total (ng/m²)		Mw		Mw
11E	74	0.10	0.05	0.05	0.09	0.01	10.33	9.61	213.49	16.30	16.30	1.13	16.05	16.05	11E	200	11a	186
12E	74	0.10	531.0	496.27	992.53	75.8	240.25	224.53	4989.66	380.89	456.66	365.27	371.37	371.37	12E	214	12a	200
13E	74	0.10	44.3	41.56	83.13	6.3	22.67	21.46	476.97	36.41	42.76	1.14	42.50	42.50	13E	228	13a	214
14E	74	0.10	554.1	522.01	1044.03	79.7	717.62	678.30	15028.81	1147.24	1226.93	262.93	1166.73	1166.73	14E	242	14a	228
15E	74	0.10	295.3	279.18	558.35	42.6	322.08	304.47	6765.99	516.49	559.11	122.10	532.08	532.08	15E	256	15a	242
16E	74	0.15	6647.3	6302.61	12605.22	962.2	8447.03	8009.04	177978.66	13586.16	14548.39	4999.42	13441.65	13441.65	16E	270	16a	256
17E	74	0.10	336.3	321.63	643.26	49.1	353.23	335.81	7462.51	569.66	618.76	363.78	538.23	538.23	17E	284	17a	270
18E	74	0.10	3483.9	3320.22	6640.44	506.9	3661.93	3480.50	81788.83	6243.42	6750.33	3457.77	5978.22	5978.22	18E	298	18a	284
19E	74	0.10	153.4	146.53	293.05	22.4	131.89	125.97	2799.36	213.69	236.06	289.56	171.96	171.96	19E	312	19a	298
20E	74	0.10	1244.7	1191.23	2382.46	181.9	866.73	829.51	18433.47	1407.14	1589.00	3939.69	716.86	716.86	20E	326	20a	312
21E	74	0.10	573.9	550.23	1100.45	84.0	370.74	355.48	7899.47	603.01	687.02	1721.03	306.02	306.02	21E	340	21a	326
22E	74	0.15	2710.1	2602.96	5205.92	397.4	1648.37	1583.18	35181.78	2685.63	3083.03	7697.89	1378.92	1378.92	22E	354	22a	340
23E	74	0.10	1356.4	1306.71	2613.42	199.5	825.46	794.08	17646.21	1347.04	1546.54	3166.70	841.09	841.09	23E	368	23a	354
24E	74	0.15	3479.6	3352.03	6704.07	511.8	2567.32	2473.23	54960.61	4195.47	4707.23	6736.25	2772.81	2772.81	24E	382	24a	368
25E	74	0.15	630.5	608.23	1216.47	92.9	551.32	531.83	11818.43	902.17	995.03	1100.18	751.46	751.46	25E	396	25a	382
26E	74	0.15	1550.8	1497.89	2995.78	228.7	1703.79	1645.61	36569.21	2791.54	3020.23	3581.97	2227.27	2227.27	26E	410	26a	396
27E	74	0.15	97.1	93.92	187.84	14.3	156.29	151.13	3358.52	256.38	270.71	17.91	266.75	266.75	27E	424	27a	410
28E	74	0.15	363.6	352.00	704.00	53.7	734.16	710.69	15793.17	1205.59	1259.33	784.92	1059.99	1059.99	28E	438	28a	424
29E	74	0.25	0.13	0.12	0.24	0.02	110.32	106.90	2375.59	181.34	181.36	2.93	180.71	180.71	29E	452	29a	438
30E	74	0.25	0.13	0.12	0.24	0.02	307.54	298.30	6628.98	506.03	506.05	2.94	505.40	505.40	30E	466	30a	452
31E	74	0.25	0.13	0.12	0.24	0.02	85.36	83.73	1194.10	91.15	91.17	2.94	90.52	90.52	31E	480	31a	466
TOTAL			24056.7	22965.62	45971.2	3509.3					36882.74	42391.99	40670.44	33368.61	33368.61			
6DE	101	0.27	2364.3	1983.87	3967.7	302.9	0.13	0.11	2.51	0.19	303.07	78.37	285.72	285.72	6de	174	6da	146
7DE	115	0.30	1363.2	1160.17	2320.3	177.1	35.81	30.47	677.17	51.69	228.82	3.07	228.14	228.14	7de	188	7da	160
8DE	129	0.25	2315.6	1994.66	3989.3	304.5	346.35	298.34	6629.63	506.09	810.62	2.62	810.04	810.04	8de	202	8da	174
9DE	185	0.39	2795.7	2433.28	4866.6	371.5	1544.92	1344.65	29881.16	2281.00	2652.50	138.64	2621.81	2621.81	9de	216	9da	188
10DE	199	0.31	205.3	180.26	360.5	27.5	172.99	151.93	3376.20	257.73	285.25	3.30	284.52	284.52	10de	230	10da	202
11DE	213	0.44	200.6	177.59	355.2	27.1	110.45	97.78	2172.62	165.86	192.98	4.69	191.94	191.94	11de	244	11da	216
12DE	227	0.57	225.5	201.02	402.0	30.7	26.83	23.91	531.43	40.57	71.26	6.18	69.89	69.89	12de	258	12da	230
13DE	241	0.49	96.6	86.64	173.3	13.2	21.49	19.28	428.48	32.71	45.94	5.27	44.77	44.77	13de	272	13da	244
14DE	255	0.97	90.9	82.02	164.0	12.5	0.49	0.44	9.76	0.75	13.27	10.64	10.91	10.91	14de	286	14da	258
TOTAL			9857.7	8299.51	16599.0	1267.1					3336.59	4603.69	252.78	4547.74	4547.74			
tph	163	0.10	0.05	0.04	0.09	0.01	0.05	0.04	0.95	0.07	0.08	1.04	-0.15	0.05	tph	194	corre.acid	166
ph	163	0.10	4300.4	4107.56	8215.12	627.1	20.39	17.44	387.64	29.50	656.70	45.15	646.70	646.70	ph	194		166
iph	163	0.10	102.2	87.41	174.82	13.3	0.05	0.04	0.95	0.07	13.42	1.04	13.19	13.19	iph	194		166
o-ph	177	0.05	161.9	140.14	280.28	21.4	1.31	1.13	25.12	1.92	23.31	4.40	22.34	22.34	o-ph	208		180
124BE	221	0.05	249.1	207.56	415.12	31.7	83.42	69.52	1544.84	117.93	149.62	1.01	149.39	149.39	124be	252		210
123BE	221	0.05	140.5	117.07	234.14	17.9	0.75	0.63	13.93	1.06	18.94	9.03	16.94	16.94	123be	252		210
135BE	221	0.05	10.8	8.99	17.96	1.4	0.03	0.02	0.46	0.04	1.41	1.05	1.18	1.18	135be	252		210
1245BE	279	0.02	15.7	12.89	25.78	2.0	0.01	0.01	0.18	0.01	1.98	0.20	1.94	1.94	1245be	310		254
12NE	213	0.05	15.6	13.77	27.55	2.1	0.03	0.02	0.49	0.04	2.14	0.54	2.02	2.02	12ne	244		216
TOTAL			5496.2	4695.44	9390.9	716.9					150.73	867.59	63.45	853.55	853.75			
PE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.02	0.23	-0.03	0.01	PE	316	corre.acid	302
SPE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.02	0.23	-0.03	0.01	SPE	316		302
IPE	241	0.08	116.4	111.20	222.41	17.0	0.04	0.04	0.85	0.06	17.04	0.93	16.84	16.84	IPE	316		302
DHE	239	0.02	25.1	23.97	47.94	3.7	26.22	25.06	609.21	45.74	49.40	128.06	21.05	21.05	DHE	314		300
ODE	253	0.06	35.1	33.63	67.26	5.1	43.12	41.26	917.41	70.03	75.17	18.59	71.05	71.05	ODE	328		314
TOTAL			176.6	168.82	337.6	25.8					115.87	141.64	148.04	108.87	108.96			
TOTAL ACIDS						5319.9					42483.9	48004.9	41134.7	36999.8	36999.1			

* Total volume	10.0 ml	Analysed volume	5.0 ml		
** Sampling area	13.1 m2				% corr./noncorr.
a: Total volume	10.0 ml	Analysed volume	1.95 ml		81
Gravimetric W (mg m²)	28.7				
# Kimwipes:	29				

Residential Outdoor (RSO)
MR 14/01

name	Ion	CL	Methanol extract: E Mass in sample (ng)	A Mass in sample (ng)	Vol correction *	Transfer to ng/m² **	DCM extract: E Mass in sample (ng/450uL)	A Mass in sample (ng/450uL)	Vol correction a	Transfer to ng/m² **	Total: Total (ng/m²)	Correction of blanks: Total mass in ave FB (ng)	Corrected total (ng/m²)	Correction with IS: Corrected total (ng/m²)
11E	74	0.10	0.05	0.05	0.08	0.01	0.05	0.05	1.03	0.10	0.11	1.13	-0.12	0.05
12E	74	0.10	88.8	80.95	161.92	16.0	33.88	31.88	703.67	68.32	85.27	358.27	6.56	6.56
13E	74	0.10	0.05	0.05	0.09	0.01	5.84	5.48	121.80	12.00	12.01	1.14	11.77	11.77
14E	74	0.10	207.5	195.40	390.80	38.5	88.87	91.00	2080.81	206.00	244.52	262.80	190.12	190.12
15E	74	0.10	118.2	109.05	218.73	21.6	63.46	58.80	1332.80	131.33	152.93	122.90	127.71	127.71
16E	74	0.15	4092.8	3880.67	7781.35	764.7	1797.37	1884.08	37658.02	3710.33	4474.98	4088.42	3440.83	3440.83
17E	74	0.10	221.4	210.44	420.89	41.5	102.29	97.25	2161.06	212.91	254.39	383.78	178.11	178.11
18E	74	0.10	2101.4	2002.68	4005.36	394.6	1108.20	1064.21	23471.52	2312.46	2707.06	3467.77	1905.40	1905.40
19E	74	0.10	295.8	283.44	566.88	55.8	81.58	77.80	1731.10	170.56	226.40	208.56	108.40	108.40
20E	74	0.10	3538.8	3387.55	6775.10	667.5	616.04	483.09	10878.93	1003.58	1740.30	3838.88	883.27	883.27
21E	74	0.10	1042.2	1580.31	3160.61	311.4	212.07	204.11	4538.73	446.67	758.28	1721.03	402.10	402.10
22E	74	0.15	8090.8	7770.61	15541.22	1531.2	892.13	886.27	19094.79	1960.06	3491.23	7087.59	1090.57	1090.57
23E	74	0.10	3958.4	3711.58	7423.16	731.3	416.82	386.29	8784.20	855.44	1586.79	3168.70	887.47	887.47
24E	74	0.15	10033.3	9665.63	19331.26	1904.6	1638.80	1462.59	32946.35	3245.95	5150.50	6730.25	3342.59	3342.59
25E	74	0.15	1558.5	1501.51	3003.02	295.9	308.65	288.70	6537.66	653.90	949.04	1100.18	722.21	722.21
26E	74	0.15	3967.0	3521.82	7043.64	753.1	1232.70	1160.80	20468.74	2006.07	3356.90	3561.97	2618.60	2618.60
27E	74	0.16	190.1	183.80	367.60	36.2	175.94	170.13	3780.75	372.49	408.71	17.81	405.00	405.00
28E	74	0.16	736.7	713.17	1426.35	140.5	1121.60	1066.75	24127.77	2377.12	2517.65	704.92	2358.39	2358.39
29E	74	0.25	0.13	0.12	0.24	0.02	161.74	178.11	3013.80	306.87	305.59	2.80	304.80	304.80
30E	74	0.25	0.13	0.12	0.24	0.02	688.78	677.71	15000.22	1403.77	1403.79	2.94	1403.18	1403.18
31E	74	0.25	0.13	0.12	0.24	0.02	0.13	0.12	2.70	0.27	0.29	2.94	-0.32	0.13
TOTAL			40733.8	39100.1	78200.2	7704.4				22304.25	30008.70	40670.44	21584.12	21584.74
6DE	101	0.27	2821.0	2460.80	4802.0	482.0	0.13	0.11	2.61	0.25	483.20	78.37	408.80	408.80
7DE	116	0.30	2052.1	1748.43	3492.9	344.1	38.17	32.40	721.02	71.12	418.24	3.07	414.60	414.60
8DE	129	0.25	3322.3	2861.02	5723.6	563.8	82.05	71.37	1505.80	158.25	720.10	2.82	718.62	718.62
9DE	165	0.38	4438.1	3863.65	7727.3	761.3	638.41	564.85	12347.91	1216.54	1977.85	130.04	1948.17	1948.17
10DE	188	0.31	217.8	180.80	361.2	37.6	120.22	108.80	2340.28	231.10	268.71	3.30	268.03	268.03
11DE	213	0.44	92.6	79.65	158.3	15.7	63.33	58.80	1245.60	122.74	138.44	4.60	137.47	137.47
12DE	227	0.57	283.4	252.01	506.2	49.8	41.06	38.60	813.38	80.13	129.91	8.16	129.63	129.63
13DE	241	0.40	87.1	78.12	156.2	15.4	28.51	23.78	828.84	82.07	97.47	5.27	68.37	68.37
14DE	255	0.87	0.48	0.44	0.9	0.09	0.40	0.44	8.78	0.86	1.05	10.04	-1.16	0.40
TOTAL			13412.4	11524.3	23048.6	2270.8				1801.23	4202.02	252.78	4148.72	4151.38
tph	163	0.10	0.05	0.04	0.09	0.01	0.05	0.04	0.85	0.09	0.10	1.04	-0.11	0.05
ph	163	0.10	1624.6	1561.28	3122.56	307.6	16.10	13.04	307.80	30.31	337.95	46.15	328.81	328.81
tph	163	0.10	546.5	408.35	808.71	82.5	0.05	0.04	0.85	0.09	82.59	1.04	82.36	82.36
o-ph	177	0.05	550.0	545.10	1090.31	107.4	1.31	1.13	25.14	2.40	109.90	4.40	106.89	106.89
124BE	221	0.05	82.7	77.23	154.47	15.2	0.00	0.02	0.40	0.05	15.20	1.01	15.06	15.06
123BE	221	0.05	404.7	387.29	774.56	76.3	0.03	0.02	0.40	0.05	76.36	0.03	74.40	74.40
135BE	221	0.05	11.8	9.84	19.69	2.0	0.00	0.02	0.40	0.05	2.00	1.05	1.79	1.79
1245BE	279	0.02	9.9	8.13	16.25	1.6	0.01	0.01	0.10	0.02	1.62	0.20	1.80	1.80
12NE	213	0.05	52.0	46.08	92.15	9.1	0.00	0.02	0.40	0.05	9.13	0.64	9.02	9.02
TOTAL			3834.5	3104.5	6209.0	611.7				33.17	644.69	60.45	631.77	631.80
PE	121	0.02	0.01	0.01	0.02	0.00	4.10	3.82	87.06	8.50	8.50	0.23	8.53	8.53
SPE	121	0.02	0.01	0.01	0.02	0.00	3.40	3.31	73.62	7.24	7.24	0.23	7.20	7.20
IPE	241	0.08	0.04	0.04	0.09	0.01	8.16	8.78	185.05	18.22	18.22	0.80	18.03	18.03
CHE	239	0.02	48.6	46.46	92.89	9.2	46.00	46.82	1040.41	102.50	111.60	126.08	85.16	85.16
CCE	253	0.08	34.8	33.35	66.70	6.6	46.40	46.33	1028.63	101.44	108.01	16.59	104.17	104.17
TOTAL			83.5	79.8	158.7	15.7				236.80	254.72	146.04	224.08	240.13
TOTAL ACIDS						10602.7				34107.0	35116.3	41134.7	26699.7	26618.2

	Mw		Mw	1F3	2F3	3F3	Average	Stdev
11E	200	11a	186	0	0.0	0.0	0.0	0.0
12E	214	12a	200	71.54	98.2	98.2	88.8	15.1
13E	228	13a	214	0.00	0.0	0.0	0.0	0.0
14E	242	14a	228	208.35	215.9	197.2	207.5	9.5
15E	256	15a	242	113.40	113.0	121.3	116.2	4.4
16E	270	16a	256	4056.10	4032.2	4191.4	4092.8	86.1
17E	284	17a	270	201.67	231.1	231.3	221.4	17.0
18E	298	18a	284	2054.55	2128.7	2121.0	2101.4	39.9
19E	312	19a	298	285.19	303.9	301.2	295.8	10.1
20E	326	20a	312	3548.11	3532.3	3537.3	3538.8	8.6
21E	340	21a	326	1008.43	1041.0	1088.3	1042.2	42.3
22E	354	22a	340	7946.60	8158.8	8085.5	8090.8	218.7
23E	368	23a	354	3730.10	4060.0	3778.9	3958.4	178.0
24E	382	24a	368	9947.45	10032.0	10220.6	10033.3	186.6
25E	396	25a	382	1533.00	1578.8	1537.0	1558.5	21.1
26E	410	26a	396	3827.60	4020.8	3916.7	3967.0	63.7
27E	424	27a	410	177.60	181.8	210.8	190.1	18.0
28E	438	28a	424	744.00	735.1	730.9	736.7	6.7
29E	452	29a	438	0	0	0.0	0.0	0.0
30E	466	30a	452	0	0	0.0	0.0	0.0
31E	480	31a	466	0	0	0.0	0.0	0.0
6de	174	6da	146	2778.4	2725.1	2960.7	2821.0	80.8
7de	188	7da	160	2070.9	2100.2	1917.0	2052.1	123.0
8de	202	8da	174	3354.1	3165.3	3447.6	3322.3	143.9
9de	216	9da	188	4483.8	4193.1	4635.5	4438.1	234.6
10de	230	10da	202	173.3	244.7	233.8	217.8	38.3
11de	244	11da	216	88.9	98.0	91.0	92.6	5.0
12de	258	12da	230	278.1	274.1	298.9	283.4	14.3
13de	272	13da	244	74.3	95.9	91.1	87.1	11.4
14de	286	14da	258	0.0	0.0	0.0	0.0	0.0
tph	194	[illegible] acid	166	0.0	0.0	0.0	0.0	0.0
ph	194		166	1630.9	1601.3	1641.7	1624.6	20.9
tph	194		166	560.0	520.7	558.9	546.5	27.5
o-ph	208		180	604.4	646.8	639.7	630.0	22.4
124be	252		216	80.7	84.1	87.3	82.7	3.4
123be	252		210	401.1	404.6	408.4	404.7	3.7
135be	252		210	11.5	11.0	12.5	11.8	0.6
1245be	316		254	8.3	11.2	8.2	9.9	1.2
12ne	244		216	48.4	54.0	51.0	52.0	3.4
PE	316	[illegible] acid	302	0.0	0.0	0.0	0.0	0.0
SPE	316		302	0.0	0.0	0.0	0.0	0.0
IPE	316		302	0.0	0.0	0.0	0.0	0.0
CHE	314		300	42.0	51.8	51.4	48.6	5.0
CCE	328		314	35.5	35.2	33.8	34.8	0.9

% corr./recov.: 78

* Total volume 10.0 ml — Analysed volume 5.0 ml
** Sampling area 10.15 m2
a Total volume 10.0 ml — Analysed volume 1.00 ml
Gravimetric W (mg m^{-2}) 83.1
\# Kompounds 21

Pharmacy Building West Indoor (PHWI)

MR 15/01

			Methanol extract				DCM extract				Total	Correction of blanks		Correction with 0.5DL					
name	Ion	DL	E Mass in sample (ng)	A Mass in sample (ng)	Vol correction *	Transfer to ng/m³ **	E Mass in sample (ng/450uL)	A Mass in sample (ng/450uL)	Vol correction *	Transfer to ng/m³ **	Total (ng/m³)	Total mass in ave FB (ng)	Corrected total (ng/m³)	Corrected total (ng/m³)		Mw		Mw
11E	74	0.10	205.0	190.62	381.24	78.2	0.05	0.05	1.03	0.21	78.45	1.13	78.07	78.07	11E	200	11a	186
12E	74	0.10	390.2	364.64	729.29	145.9	190.31	177.86	3952.47	790.49	936.35	385.27	805.36	805.36	12E	214	12a	200
13E	74	0.10	20.3	19.02	38.03	7.6	30.67	28.78	639.61	127.92	135.53	1.14	135.14	135.14	13E	228	13a	214
14E	74	0.10	354.2	333.73	667.46	133.5	963.77	926.86	20596.85	4119.37	4252.86	262.93	4163.47	4163.47	14E	242	14a	228
15E	74	0.10	169.7	160.46	320.93	64.2	500.85	473.46	10521.43	2104.29	2168.47	122.10	2126.96	2126.96	15E	256	15a	242
16E	74	0.15	3680.7	3489.85	6979.69	1395.9	9373.41	8887.38	197497.35	39499.47	40895.41	4999.42	39195.61	39195.61	16E	270	16a	256
17E	74	0.10	171.8	163.32	326.64	65.3	504.12	479.27	10650.45	2130.09	2195.42	363.78	2071.73	2071.73	17E	284	17a	270
18E	74	0.10	1514.5	1443.35	2886.69	577.3	4474.14	4263.94	94754.32	18950.86	19528.20	3487.77	18342.36	18342.36	18E	298	18a	284
19E	74	0.10	105.8	101.04	202.09	40.4	175.29	167.43	3720.58	744.12	784.53	289.56	686.09	686.09	19E	312	19a	298
20E	74	0.10	879.4	841.82	1683.24	336.6	726.61	695.41	15453.52	3090.70	3427.35	3939.69	2067.66	2067.66	20E	326	20a	312
21E	74	0.10	445.6	427.27	854.55	170.9	329.32	315.76	7016.96	1403.39	1574.30	1721.03	969.15	969.15	21E	340	21a	326
22E	74	0.15	2206.8	2121.46	4242.93	848.6	1463.74	1405.85	31241.06	6248.22	7096.80	7697.89	4479.52	4479.52	22E	354	22a	340
23E	74	0.10	1125.2	1082.41	2164.83	433.0	769.07	739.61	16440.32	3288.06	3721.03	3186.70	2637.55	2637.55	23E	368	23a	354
24E	74	0.15	3401.3	3276.67	6553.35	1310.7	2422.57	2333.78	51861.85	10372.37	11683.04	6738.25	5712.03	5712.03	24E	382	24a	368
25E	74	0.15	602.9	581.61	1163.22	232.6	576.63	556.25	12361.07	2472.21	2704.86	1100.18	2330.79	2330.79	25E	396	25a	382
27E	74	0.15	1642.6	1586.48	3172.95	634.6	1620.78	1565.42	34787.13	6957.43	7592.02	3581.97	6374.14	6374.14	26E	410	26a	396
28E	74	0.15	70.0	67.67	135.34	27.1	169.45	163.65	3641.19	728.24	755.31	17.91	749.22	749.22	27E	424	27a	410
29E	74	0.25	361.5	349.92	699.85	140.0	715.59	692.72	15393.74	3078.75	3218.72	764.92	2958.65	2958.65	28E	438	28a	424
30E	74	0.25	0.13	0.12	0.24	0.05	91.70	88.86	1974.77	394.95	395.00	2.93	394.00	394.00	29E	452	29a	438
31E	74	0.25	0.13	0.12	0.24	0.05	226.53	219.73	4882.81	976.56	976.61	2.94	975.61	975.61	30E	466	30a	452
TOTAL			17349.8	16801.5	33203.0	6640.6	0.13	0.12	2.70	0.54	0.59	2.94	-0.41	0.13	31E	480	31a	466
										107478.24	114118.85	40670.44	100290.90	100291.44				
6DE	101	0.27	1855.4	1389.05	2778.1	555.6	414.55	347.84	7729.76	1545.96	2101.58	78.37	2074.93	2074.93	6de	174	6da	148
7DE	115	0.30	544.2	463.19	926.4	185.3	302.38	257.35	5718.63	1143.77	1329.04	3.07	1326.00	1326.00	7de	188	7da	160
8DE	129	0.25	835.3	719.51	1439.0	287.8	712.27	613.54	13634.24	2726.85	3014.65	2.62	3013.76	3013.76	8de	202	8da	174
9DE	185	0.39	1764.3	1535.59	3071.2	614.2	1732.46	1507.68	33506.40	6701.68	7315.92	138.64	7268.78	7268.78	9de	216	9da	186
10DE	199	0.31	216.1	189.78	379.6	75.9	156.65	137.58	3057.24	611.45	687.36	3.30	686.24	686.24	10de	230	10da	202
11DE	213	0.44	128.8	114.04	228.1	45.6	135.38	119.84	2663.17	532.63	578.25	4.69	576.66	576.66	11de	244	11da	216
12DE	227	0.57	208.7	186.04	372.1	74.4	83.20	74.17	1648.23	329.65	404.06	6.18	401.96	401.96	12de	258	12da	230
13DE	241	0.49	0.24	0.22	0.4	0.09	48.61	43.61	969.06	193.81	193.90	5.27	192.11	192.11	13de	272	13da	244
14DE	255	0.97	0.49	0.44	0.9	0.18	34.43	31.06	690.12	138.02	138.20	10.64	134.58	134.58	14de	286	14da	258
TOTAL			5353.6	4597.9	9195.7	1839.1				13923.61	15762.96	252.78	15677.01	15677.01				
tph	163	0.10	340.8	291.58	583.2	116.6	21.35	18.27	405.90	81.18	197.81	1.04	197.46	197.46	tph	194	corre.acid	166
ph	163	0.10	2879.6	2292.89	4585.8	917.2	37.44	32.04	711.96	142.40	1059.55	45.15	1044.20	1044.20	ph	194		166
iph	163	0.10	324.2	277.37	554.7	110.9	6.64	5.68	126.30	25.26	136.21	1.04	135.66	135.66	iph	194		166
o-ph	177	0.05	303.7	262.81	525.6	105.1	15.43	13.35	296.69	59.34	164.46	4.40	162.97	162.97	o-ph	208		180
124BE	221	0.05	50.8	42.30	84.6	16.9	9.30	7.75	172.24	34.45	51.37	1.01	51.03	51.03	124be	252		210
123BE	221	0.05	177.7	148.09	296.2	59.2	0.03	0.02	0.48	0.09	59.33	9.03	56.26	56.26	123be	252		210
135BE	221	0.05	0.03	0.02	0.0	0.01	3.07	2.56	56.82	11.36	11.37	1.05	11.02	11.02	135be	252		210
1245BE	279	0.02	3.6	2.94	5.9	1.2	0.01	0.01	0.16	0.04	1.21	0.20	1.15	1.15	1245be	310		254
12NE	213	0.05	5.5	4.89	9.8	2.0	0.03	0.02	0.49	0.10	2.05	0.54	1.87	1.87	12ne	244		216
TOTAL			3885.9	3322.9	6645.8	1329.2				354.21	1683.37	63.45	1661.80	1661.80				
PE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.22	4.94	0.99	0.99	0.23	0.91	0.91	PE	316	corre.acid	302
SPE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.22	4.94	0.99	0.99	0.23	0.91	0.91	SPE	316		302
IPE	241	0.06	524.6	501.31	1002.63	200.5	41.19	915.34	20340.99	4068.20	4268.72	0.93	4268.41	4268.41	IPE	316		302
DHE	239	0.02	66.0	63.09	126.17	25.2	77.06	1712.69	38064.28	7612.86	7638.09	126.06	7594.55	7594.55	DHE	314		300
ODE	253	0.06	67.1	64.21	128.41	25.7	80.99	1799.76	39994.61	7998.92	8024.61	18.59	8018.28	8018.28	ODE	328		314
TOTAL			657.7	628.6	1257.2	251.4				19681.95	19933.40	148.04	19883.07	19883.07				
TOTAL ACIDS						19060.4												
										141438.2	151498.6	41134.7	137512.8	137513.3				

* Total volume 10.0 ml Analysed volume 5.0 ml

** Sampling area 5.0 m2

a: Total volume 10.0 ml Analysed volume 1.47 ml

Gravimetric W (mg m³) 55.2

Kimwipes: 17

% corr./noncorr. 91

Pharmacy Building West Outdoor (PHWO)

MR 16/01

			Methanol extract				DCM extract				Total	Correction of blanks		Correction with 0.5DL				
name	Ion	DL	E Mass in sample (ng)	A Mass in sample (ng)	Vol correction *	Transfer to ng/m³ **	E Mass in sample (ng/450uL)	A Mass in sample (ng/450uL)	Vol correction *	Transfer to ng/m³ **	Total (ng/m³)	Total mass in ave FB (ng)	Corrected total (ng/m³)	Corrected total (ng/m³)		Mw		Mw
11E	74	0.10	0.05	0.05	0.09	0.02	0.05	0.05	1.03	0.18	0.20	1.13	-0.14	0.05	11E	200	11a	186
12E	74	0.10	139.7	130.58	261.16	45.8	18.72	17.50	388.66	68.22	114.04	385.27	-0.87	0.05	12E	214	12a	200
13E	74	0.10	0.0	0.00	0.00	0.0	0.05	0.05	1.04	0.18	0.18	1.14	-0.16	0.05	13E	228	13a	214
14E	74	0.10	118.5	111.88	223.35	39.2	47.50	44.75	994.56	174.48	213.67	262.93	135.25	135.25	14E	242	14a	228
15E	74	0.10	0.0	0.00	0.00	0.0	32.41	30.64	680.91	119.46	119.46	122.10	83.04	83.04	15E	256	15a	242
16E	74	0.15	2008.7	1904.54	3809.07	668.3	963.99	914.00	20311.17	3563.36	4231.62	4999.42	2740.57	2740.57	16E	270	16a	256
17E	74	0.10	120.2	114.30	228.60	40.1	39.74	37.78	839.50	147.28	187.39	383.78	78.89	78.89	17E	284	17a	270
18E	74	0.10	1020.7	972.79	1945.58	341.3	806.66	482.88	10730.60	1882.56	2223.89	3487.77	1183.65	1183.65	18E	298	18a	284
19E	74	0.10	104.3	99.65	199.30	35.0	24.62	23.52	522.63	91.69	126.65	289.56	40.29	40.29	19E	312	19a	298
20E	74	0.10	1718.1	1644.30	3288.61	576.9	235.00	224.91	4997.93	876.63	1453.78	3939.69	278.78	278.78	20E	326	20a	312
21E	74	0.10	843.7	808.98	1617.97	283.9	87.70	84.06	1868.53	327.81	611.67	1721.03	96.38	96.38	21E	340	21a	326
22E	74	0.15	4133.4	3969.94	7939.89	1393.0	443.44	425.90	9464.54	1660.45	3053.41	7697.89	757.55	757.55	22E	354	22a	340
23E	74	0.10	1886.3	1814.52	3629.05	636.7	206.29	198.45	4409.89	773.67	1410.34	3186.70	459.92	459.92	23E	368	23a	354
24E	74	0.15	4451.5	4268.39	8578.78	1504.7	635.46	612.17	13603.84	2386.64	3891.34	8736.25	1265.19	1265.19	24E	382	24a	368
25E	74	0.15	563.7	543.81	1087.62	190.8	105.09	101.37	2252.74	395.22	586.03	1100.18	257.90	257.90	25E	396	25a	382
26E	74	0.15	1258.3	1215.32	2430.63	426.4	457.19	441.57	9812.76	1721.54	2147.96	3581.97	1079.66	1079.66	26E	410	26a	396
27E	74	0.15	54.0	52.17	104.34	18.3	46.26	44.75	994.44	174.46	192.77	17.91	187.43	187.43	27E	424	27a	410
28E	74	0.15	233.5	226.07	452.15	79.3	309.49	299.60	6657.82	1168.04	1247.36	764.92	1019.23	1019.23	28E	438	28a	424
29E	74	0.25	0.13	0.12	0.24	0.04	0.13	0.12	2.69	0.47	0.51	2.93	-0.36	0.13	29E	452	29a	438
30E	74	0.25	0.13	0.12	0.24	0.04	95.12	92.26	2050.28	359.70	359.74	2.94	358.66	358.66	30E	466	30a	452
31E	74	0.25	0.13	0.12	0.24	0.04	0.13	0.12	2.70	0.47	0.52	2.94	-0.36	0.13	31E	480	31a	466
TOTAL			18655.2		35794.9	6279.8					15892.71	22172.52	40670.44	10042.74	10045.02			
6DE	191	0.27	0.13	0.11	0.23	0.04	0.13	0.11	2.51	0.44	0.48	78.37	-22.69	0.13	6de	174	6da	148
7DE	115	0.30	0.15	0.13	0.25	0.04	11.93	10.15	225.64	39.59	39.63	3.07	36.72	36.72	7de	188	7da	160
8DE	129	0.25	0.13	0.11	0.22	0.04	0.13	0.11	2.40	0.42	0.46	2.62	-0.32	0.13	8de	202	8da	174
9DE	185	0.29	468.6	425.26	850.52	149.2	0.19	0.17	3.74	0.66	149.87	138.64	108.52	108.52	9de	216	9da	188
10DE	199	0.31	0.16	0.14	0.27	0.05	0.16	0.14	3.03	0.53	0.58	3.30	-0.40	0.16	10de	230	10da	202
11DE	213	0.44	0.22	0.19	0.39	0.07	0.22	0.19	4.30	0.75	0.82	4.69	-0.58	0.22	11de	244	11da	216
12DE	227	0.57	0.29	0.26	0.51	0.09	0.29	0.26	5.67	0.99	1.08	6.18	-0.76	0.29	12de	258	12da	230
13DE	241	0.49	0.24	0.22	0.44	0.08	0.24	0.22	4.84	0.85	0.92	5.27	-0.65	0.24	13de	272	13da	244
14DE	255	0.97	0.49	0.44	0.88	0.15	0.49	0.44	9.76	1.71	1.87	10.64	-1.31	0.49	14de	286	14da	258
TOTAL			490.4	426.8	853.7	149.8					45.95	193.72	252.78	120.33	148.89			
iph	163	0.10	0.05	0.04	0.09	0.02	0.05	0.04	0.95	0.17	0.18	1.04	-0.13	0.05	iph	194	corra.acid	166
ph	163	0.10	621.8	532.05	1064.11	186.7	25.39	21.72	482.72	84.69	271.37	45.15	257.91	257.91	ph	194		166
iph	163	0.10	0.05	0.04	0.09	0.02	0.05	0.04	0.95	0.17	0.18	1.04	-0.13	0.05	iph	194		166
o-ph	177	0.05	79.1	66.44	136.87	24.0	0.03	0.02	0.48	0.08	24.10	4.40	22.79	22.79	o-ph	208		180
124BE	221	0.05	0.03	0.02	0.04	0.01	0.03	0.02	0.48	0.08	0.09	1.01	-0.21	0.03	124be	252		210
123BE	221	0.05	71.4	59.49	118.99	20.9	0.03	0.02	0.48	0.08	20.98	9.03	18.26	18.26	123be	252		210
135BE	221	0.05	0.03	0.02	0.04	0.01	0.03	0.02	0.48	0.08	0.09	1.05	-0.22	0.03	135be	252		210
1245BE	279	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.18	0.03	0.03	0.20	-0.02	0.01	1245be	310		254
12NE	213	0.05	0.03	0.02	0.04	0.01	0.03	0.02	0.49	0.09	0.09	0.54	-0.07	0.03	12ne	244		216
TOTAL			772.5	660.1	1320.3	231.6					65.47	317.10	63.45	299.17	299.14			
PE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.04	0.04	0.23	-0.03	0.01	PE	316	corra.acid	302
SPE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.04	0.04	0.23	-0.03	0.01	SPE	316		302
IPE	241	0.08	0.04	0.04	0.08	0.01	0.04	0.04	0.85	0.15	0.18	0.93	-0.11	0.04	IPE	316		302
DHE	239	0.02	189.4	160.88	321.96	55.5	31.66	30.25	672.27	117.84	181.44	128.06	143.25	143.25	DHE	314		300
ODE	253	0.06	0.03	0.03	0.06	0.01	11.14	10.66	236.95	41.57	41.58	16.59	36.04	36.04	ODE	328		314
TOTAL			189.5	161.1	322.1	55.5					159.74	223.27	148.04	179.12	179.25			
TOTAL ACIDS						6724.7					19193.8	22908.6	41134.7	10840.4	10672.4			

* Total volume	10.0 ml	Analysed volume	5.0 ml		
** Sampling area	5.7 m2			% corr./noncorr.	
a: Total volume	10.0 ml	Analysed volume	1.99 ml	46.6	
Gravimetric W (mg m⁻³)	107.2				
# Kimwipes:	17				

South Riverdale Indoor (SRI)

MR 15/01

			Methanol extract				DCM extract				Total	Correction of blanks		Correction with 0.5DL				
name	Ion	DL	E Mass in sample (ng)	A Mass in sample (ng)	Vol correction *	Transfer to ng/m² **	E Mass in sample (ng/450uL)	A Mass in sample (ng/450uL)	Vol correction *	Transfer to ng/m² **	Total (ng/m²)	Total mass in sve FB (ng)	Corrected total (ng/m²)	Corrected total (ng/m²)		Mw		Mw
11E	74	0.10	0.05	0.05	0.09	0.01	2.40	2.23	49.63	4.24	4.25	1.13	4.10	4.10	11E	200	11a	186
12E	74	0.10	1107.4	1034.99	2069.86	176.9	91.91	85.90	1906.79	163.14	340.07	365.27	287.38	287.38	12E	214	12a	200
13E	74	0.10	0.0	0.00	0.00	0.0	6.00	5.63	125.17	10.70	10.70	1.14	10.54	10.54	13E	228	13a	214
14E	74	0.10	619.0	583.18	1166.36	99.7	152.74	143.91	3197.89	273.32	373.01	262.93	337.06	337.06	14E	242	14a	228
15E	74	0.10	163.8	154.82	309.65	26.5	69.20	65.42	1453.69	124.25	150.71	122.10	134.01	134.01	15E	256	15a	242
16E	74	0.15	2955.6	2802.33	5604.65	479.0	1157.40	1097.39	24366.36	2084.30	2563.33	4999.42	1879.65	1879.65	16E	270	16a	256
17E	74	0.10	158.1	150.34	300.69	25.7	89.19	84.79	1884.33	161.05	186.75	363.78	137.01	137.01	17E	284	17a	270
18E	74	0.10	1259.3	1200.14	2400.27	205.2	943.67	899.34	19965.31	1706.15	1913.30	3487.77	1436.34	1436.34	18E	298	18a	284
19E	74	0.10	78.8	73.35	146.70	12.5	46.36	44.25	983.95	84.10	96.64	259.56	57.04	57.04	19E	312	19a	298
20E	74	0.10	610.8	584.59	1169.17	99.9	435.36	416.66	9259.13	791.36	891.31	3939.69	352.55	352.55	20E	326	20a	312
21E	74	0.10	245.3	235.22	470.45	40.2	209.21	200.59	4457.56	380.99	421.20	1721.03	185.84	185.84	21E	340	21a	326
22E	74	0.15	1085.5	1042.59	2085.17	178.2	1092.37	1049.17	23314.82	1992.72	2170.94	7697.89	1118.24	1118.24	22E	354	22a	340
23E	74	0.10	460.8	443.27	886.54	75.8	528.22	508.13	11291.75	965.11	1040.88	3166.70	605.09	605.09	23E	368	23a	354
24E	74	0.15	1093.8	1053.70	2107.41	180.1	1842.26	1582.07	35157.21	3004.89	3185.01	8738.25	1890.04	1890.04	24E	382	24a	368
25E	74	0.15	179.3	172.98	345.97	29.6	304.97	294.19	6537.49	558.76	588.33	1100.18	437.88	437.88	25E	396	25a	382
26E	74	0.15	415.3	401.12	802.25	68.6	924.66	893.08	19846.30	1696.26	1764.83	3581.97	1274.99	1274.99	26E	410	26a	396
27E	74	0.15	0.08	0.07	0.15	0.01	48.16	47.54	1056.48	90.30	90.31	17.91	87.86	87.86	27E	424	27a	410
28E	74	0.15	0.08	0.07	0.15	0.01	328.25	317.76	7061.34	603.53	603.55	784.92	498.84	498.84	28E	438	28a	424
29E	74	0.25	0.13	0.12	0.24	0.02	17.33	16.79	373.16	31.89	31.91	2.93	31.51	31.51	29E	452	29a	438
30E	74	0.25	0.13	0.12	0.24	0.02	41.81	40.56	901.26	77.03	77.05	2.94	76.65	76.65	30E	466	30a	452
31E	74	0.25	0.13	0.12	0.24	0.02	0.13	0.12	2.70	0.23	0.25	2.94	-0.15	0.13	31E	480	31a	466
TOTAL			10431.5	9933.2	19866.4	1698.0				14606.35	16504.33	40670.44	10942.56	10942.84				
6DE	101	0.27	990.8	831.35	1662.70	142.1	0.13	0.11	2.51	0.21	142.33	78.37	131.61	131.61	6de	174	6da	146
7DE	115	0.30	70.4	59.95	119.90	10.2	0.15	0.13	2.82	0.24	10.49	3.07	10.07	10.07	7de	188	7da	160
8DE	129	0.25	505.9	435.75	871.51	74.5	5.46	4.70	104.56	8.94	83.42	2.62	83.07	83.07	8de	202	8da	174
9DE	165	0.39	1060.1	922.70	1845.41	157.7	48.01	41.79	926.63	79.37	237.10	138.64	218.14	218.14	9de	216	9da	188
10DE	199	0.31	0.16	0.14	0.27	0.02	5.24	4.60	102.23	8.74	8.76	3.30	8.31	8.31	10de	230	10da	202
11DE	213	0.44	0.22	0.19	0.39	0.03	0.22	0.19	4.30	0.37	0.40	4.69	-0.24	0.22	11de	244	11da	216
12DE	227	0.57	0.29	0.26	0.51	0.04	0.29	0.26	5.67	0.48	0.53	6.18	-0.32	0.29	12de	258	12da	230
13DE	241	0.49	0.24	0.22	0.44	0.04	4.62	4.14	92.03	7.87	7.90	5.27	7.18	7.18	13de	272	13da	244
14DE	255	0.87	0.48	0.44	0.88	0.08	0.49	0.44	9.76	0.83	0.91	10.64	-0.55	0.49	14de	286	14da	258
TOTAL			2628.6	2251.0	4502.0	384.8				107.05	491.64	252.78	457.27	459.37				
iph	163	0.10	0.05	0.04	0.09	0.01	0.05	0.04	0.95	0.08	0.09	1.04	-0.05	0.05	iph	194	corre.acid	166
ph	163	0.10	521.3	446.05	892.10	76.2	1.34	1.15	25.55	2.18	78.43	45.15	72.26	72.26	ph	194		166
iph	163	0.10	0.0	0.00	0.00	0.0	0.05	0.04	0.95	0.08	0.08	1.04	-0.06	0.05	iph	194		166
o-ph	177	0.05	57.8	49.96	99.97	8.5	0.03	0.02	0.48	0.04	8.59	4.40	7.98	7.98	o-ph	208		180
124BE	221	0.05	33.1	27.60	55.20	4.7	0.03	0.02	0.46	0.04	4.76	1.01	4.62	4.62	124be	252		210
123BE	221	0.05	34.6	28.85	57.70	4.9	0.03	0.02	0.46	0.04	4.97	9.03	3.74	3.74	123be	252		210
135BE	221	0.05	0.03	0.02	0.04	0.00	0.03	0.02	0.46	0.04	0.04	1.05	-0.10	0.03	135be	252		210
1245BE	279	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.18	0.02	0.02	0.20	-0.01	0.01	1245be	310		254
12NE	213	0.05	0.03	0.02	0.04	0.00	0.03	0.02	0.49	0.04	0.05	0.54	-0.03	0.03	12ne	244		216
TOTAL			646.9	552.6	1105.2	94.5				2.56	97.02	63.45	88.35	88.78				
PE	121	0.02	0.01	0.01	0.02	0.00	2.08	1.99	44.21	3.78	3.78	0.23	3.75	3.75	PE	316	corre.acid	302
SPE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.02	0.23	-0.01	0.01	SPE	316		302
IPE	241	0.08	0.04	0.04	0.08	0.01	0.04	0.04	0.85	0.07	0.08	0.93	-0.05	0.04	IPE	316		302
DHE	239	0.02	26.7	25.52	51.04	4.4	20.43	19.52	433.79	37.06	41.44	126.06	23.93	23.93	DHE	314		300
ODE	253	0.06	43.0	41.16	82.36	7.0	40.50	38.78	861.67	73.65	80.69	18.59	78.14	78.14	ODE	328		314
TOTAL			69.8	66.8	133.5	11.4				114.59	126.00	148.04	105.76	103.87				
TOTAL ACIDS						2196.6				15030.6	17219.2	41134.7	11593.9	11596.8				

* Total volume	10.0 ml	Analysed volume	5.0 ml		
** Sampling area	11.70 m2				
a: Total volume	10.0 ml	Analysed volume	1.58 ml		
Gravimetric W (mg m²)	NA				
# Kimwipes:	16				

%corr./noncorr.
67.3

South Riverdale Outdoor (SRO)
MR 15/01

			Methanol extract				DCM extract				Total	Correction of blanks		Correction with 0.5DL				
name	Ion	DL	E Mass in sample (ng)	A Mass in sample (ng)	Vol correction *	Transfer to ng/m² **	E Mass in sample (ng/450uL)	A Mass in sample (ng/450uL)	Vol correction *	Transfer to ng/m² **	Total (ng/m²)	Total mass in ave FB (ng)	Corrected total (ng/m²)	Corrected total (ng/m²)		Mw		Mw
11E	74	0.10	0.05	0.05	0.09	0.01	0.05	0.05	1.03	0.11	0.12	1.13	-0.14	0.05	11E	200	11a	186
12E	74	0.10	72.3	67.80	135.19	14.5	36.33	33.96	754.57	80.70	95.16	385.27	4.51	4.51	12E	214	12a	200
13E	74	0.10	0.0	0.00	0.00	0.0	0.05	0.05	1.04	0.11	0.11	1.14	-0.16	0.05	13E	228	13a	214
14E	74	0.10	216.4	203.90	407.80	43.6	88.31	83.20	1848.83	197.74	241.35	262.93	179.49	179.49	14E	242	14a	228
15E	74	0.10	119.9	113.36	226.73	24.2	52.36	49.50	1099.93	117.64	141.89	122.10	113.16	113.16	15E	256	15a	242
16E	74	0.15	5629.9	5527.63	11055.25	1182.4	1319.42	1251.01	27800.18	2973.28	4155.66	4999.42	2979.33	2979.33	16E	270	16a	256
17E	74	0.10	208.5	198.21	396.42	42.4	84.59	81.41	1364.56	145.94	188.34	363.78	102.74	102.74	17E	284	17a	270
18E	74	0.10	1747.8	1665.73	3331.45	356.3	638.81	608.80	13528.90	1446.94	1803.25	3487.77	962.59	962.59	18E	298	18a	284
19E	74	0.10	202.5	193.38	386.76	41.4	83.40	81.90	708.93	75.82	117.19	289.56	49.05	49.05	19E	312	19a	298
20E	74	0.10	2032.1	1944.84	3889.67	416.0	231.95	221.98	4932.99	527.59	943.60	3939.69	16.62	16.62	20E	326	20a	312
21E	74	0.10	882.4	846.02	1692.04	181.0	105.71	101.35	2252.33	240.89	421.86	1721.03	16.91	16.91	21E	340	21a	326
22E	74	0.15	3681.3	3727.80	7455.59	797.4	459.38	441.21	9804.61	1048.52	1846.01	7697.89	34.74	34.74	22E	354	22a	340
23E	74	0.10	1693.3	1628.85	3257.70	348.4	210.10	202.11	4491.35	480.36	828.77	3166.70	78.96	78.96	23E	368	23a	354
24E	74	0.15	4166.7	4013.97	8027.94	858.6	680.54	655.60	14568.92	1558.17	2416.76	8738.25	360.72	360.72	24E	382	24a	368
25E	74	0.15	603.8	582.41	1164.83	124.6	118.18	114.00	2533.33	270.94	395.53	1100.18	136.66	136.66	25E	396	25a	382
26E	74	0.15	1566.0	1533.75	3067.50	328.1	422.39	407.96	9065.83	969.61	1297.66	3581.97	454.86	454.86	26E	410	26a	396
27E	74	0.15	70.2	67.66	135.72	14.5	42.56	41.17	914.93	97.85	112.37	17.91	108.16	108.16	27E	424	27a	410
28E	74	0.15	355.1	343.79	687.58	73.5	258.40	250.14	5558.58	594.50	668.04	784.92	468.06	468.06	28E	438	28a	424
29E	74	0.25	0.13	0.12	0.24	0.03	0.13	0.12	2.69	0.29	0.31	2.93	-0.38	0.13	29E	452	29a	438
30E	74	0.25	0.13	0.12	0.24	0.03	93.50	90.70	2015.44	215.56	215.56	2.94	214.89	214.89	30E	466	30a	452
31E	74	0.25	0.13	0.12	0.24	0.03	0.13	0.12	2.70	0.29	0.31	2.94	-0.38	0.13	31E	480	31a	466
TOTAL			23670.6	22659.5	45319.0	4847.0				11042.96	15889.91	40670.44	6320.40	6321.80				
6DE	101	0.27	535.2	449.09	898.2	96.1	0.13	0.11	2.51	0.27	96.33	78.37	77.89	77.89	6de	174	6da	146
7DE	115	0.30	453.5	385.99	772.0	82.6	59.01	50.22	1116.07	119.37	201.93	3.07	201.21	201.21	7de	188	7da	160
8DE	129	0.25	566.6	488.04	976.1	104.4	0.13	0.11	2.40	0.26	104.65	2.62	104.03	104.03	8de	202	8da	174
9DE	185	0.39	740.5	644.50	1289.0	137.9	122.82	106.90	2375.62	254.08	391.94	136.64	359.32	359.32	9de	216	9da	188
10DE	199	0.31	0.16	0.14	0.3	0.03	0.16	0.14	3.03	0.32	0.35	3.30	-0.42	0.16	10de	230	10da	202
11DE	213	0.44	0.22	0.19	0.4	0.04	16.19	14.33	318.47	34.06	34.10	4.69	33.00	33.00	11de	244	11da	216
12DE	227	0.57	0.29	0.26	0.5	0.05	0.29	0.26	5.67	0.61	0.66	6.18	-0.79	0.29	12de	258	12da	230
13DE	241	0.49	132.1	118.52	237.0	25.4	19.13	17.16	381.34	40.79	66.14	5.27	64.90	64.90	13de	272	13da	244
14DE	255	0.97	0.0	0.00	0.0	0.0	0.49	0.44	9.76	1.04	1.04	10.64	-1.46	0.49	14de	286	14da	258
TOTAL			2428.6	2086.7	4173.4	446.4				450.79	897.14	252.78	837.67	841.27				
tph	163	0.10	0.05	0.04	0.09	0.01	0.09	0.07	1.63	0.17	0.18	1.04	-0.06	0.05	tph	194	corre.acid	166
ph	163	0.10	1147.2	961.62	1963.23	210.0	19.58	16.76	372.36	39.82	249.80	45.15	239.17	239.17	ph	194		166
iph	163	0.10	115.9	99.15	198.31	21.2	0.09	0.07	1.63	0.17	21.38	1.04	21.14	21.14	iph	194		166
o-ph	177	0.05	294.8	255.08	510.15	54.6	1.33	1.15	25.67	2.75	57.31	4.40	56.27	56.27	o-ph	208		180
124BE	221	0.05	46.2	38.48	76.97	8.2	0.04	0.03	0.77	0.08	8.31	1.01	8.08	8.08	124be	252		210
123BE	221	0.05	117.9	96.22	196.43	21.0	0.04	0.03	0.77	0.08	21.09	9.03	18.97	18.97	123be	252		210
135BE	221	0.05	6.7	5.59	11.18	1.2	0.04	0.03	0.77	0.08	1.28	1.05	1.03	1.03	135be	252		210
1245BE	279	0.02	0.01	0.01	0.02	0.00	0.02	0.01	0.30	0.03	0.03	0.20	-0.01	0.01	1245be	310		254
12NE	213	0.05	0.03	0.02	0.04	0.00	0.04	0.04	0.87	0.09	0.10	0.54	-0.03	0.03	12ne	244		216
TOTAL			1728.7	1478.2	2956.4	316.2				43.29	359.48	63.45	344.56	344.74				
PE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.02	0.23	-0.03	0.01	PE	316	corre.acid	302
SPE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.02	0.23	-0.03	0.01	SPE	316		302
IPE	241	0.08	0.04	0.04	0.08	0.01	0.04	0.04	0.85	0.09	0.10	0.93	-0.12	0.04	IPE	316		302
DHE	239	0.02	26.8	25.59	51.18	5.5	21.06	20.12	447.05	47.81	53.29	128.06	23.16	23.16	DHE	314		300
ODE	253	0.06	0.0	0.00	0.00	0.0	10.99	10.52	233.76	25.00	25.00	18.59	20.63	20.63	ODE	328		314
TOTAL			26.8	25.6	51.3	5.5				72.95	78.44	148.04	43.60	43.84				
TOTAL ACIDS						5615.0				11610.0	17225.0	41134.7	7546.2	7551.7				

* Total volume	10.0 ml	Analysed volume	5.0 ml		%corr./noncorr
** Sampling area	9.35 m2				43.8
a: Total volume	10.0 ml	Analysed volume	1.13 ml		
Gravimetric W (mg m²)	89.8				
# Kimwipes:	22				

Jolly's Restaurant Indoor (JRI)
MR 22/01

			Methanol extract				DCM extract				Total	Correction with blanks		Correction with 0.5DL				
name	Ion	DL	E Mass in sample (ng)	A Mass in sample (ng)	Vol correction *	Transfer to ng/m² **	E Mass in sample (ng/450uL)	A Mass in sample (ng/450uL)	Vol correction *	Transfer to ng/m² **	Total (ng/m²)	Total mass in ave FB (ng)	Corrected total (ng/m²)	Corrected total (ng/m²)		Mw		Mw
11E	74	0.10	0.05	0.05	0.09	0.02	0.05	0.05	1.03	0.21	0.23	1.13	0.09	0.09	11E	200	11a	186
12E	74	0.10	564.1	545.90	1091.80	218.4	61.56	57.53	1278.44	255.69	474.05	365.27	427.81	427.81	12E	214	12a	200
13E	74	0.10	0.05	0.05	0.09	0.02	0.05	0.05	1.04	0.21	0.23	1.14	0.09	0.09	13E	228	13a	214
14E	74	0.10	1253.8	1181.28	2362.56	472.5	195.17	183.88	4086.20	817.24	1289.75	262.93	1258.20	1258.20	14E	242	14a	228
15E	74	0.10	729.6	689.72	1379.44	275.9	88.04	84.17	1870.46	374.09	649.98	182.58	628.07	628.07	15E	256	15a	242
16E	74	0.15	12104.0	11478.35	22952.69	4590.5	1643.91	1558.67	34637.12	6927.42	11517.96	4999.42	10918.03	10918.03	16E	270	16a	256
17E	74	0.10	5268.4	5027.66	10055.36	2011.1	74.74	71.05	1578.94	315.79	2326.86	363.78	2263.21	2263.21	17E	284	17a	270
18E	74	0.10	3678.8	3456.27	6916.55	1383.3	629.52	599.95	13332.11	2666.42	4049.73	3467.77	3631.20	3631.20	18E	298	18a	284
19E	74	0.10	2657.6	2536.36	5078.76	1015.4	29.18	27.87	619.35	123.87	1139.22	259.56	1104.48	1104.48	19E	312	19a	298
20E	74	0.10	2478.0	2369.63	4739.26	947.9	160.90	153.99	3422.09	684.42	1632.27	3939.69	1159.51	1159.51	20E	326	20a	312
21E	74	0.10	1310.8	1256.59	2513.17	502.6	85.06	81.56	1812.86	362.57	865.21	1721.03	658.68	658.68	21E	340	21a	326
22E	74	0.15	6011.3	5773.54	11547.07	2309.4	309.78	297.53	6611.81	1322.36	3631.78	7897.89	2706.03	2706.03	22E	354	22a	340
23E	74	0.10	3264.1	3159.13	6318.26	1263.7	154.49	148.81	3302.51	660.50	1924.15	3166.70	1541.75	1541.75	23E	368	23a	354
24E	74	0.15	9078.8	8743.93	17487.86	3497.6	466.91	449.80	9995.58	1999.12	5496.69	8738.25	4448.10	4448.10	24E	382	24a	368
25E	74	0.15	1522.4	1468.60	2937.19	587.4	67.67	64.57	1879.25	375.85	963.29	1100.18	831.27	831.27	25E	396	25a	382
26E	74	0.15	4224.5	4080.23	8160.46	1632.1	254.08	245.40	5453.36	1090.67	2722.76	3561.97	2292.93	2292.93	26E	410	26a	396
27E	74	0.15	138.7	134.14	268.28	53.7	12.41	12.00	266.70	53.34	107.00	1.76	106.79	106.79	27E	424	27a	410
28E	74	0.15	843.1	816.16	1632.32	326.5	95.21	92.16	2048.07	409.61	736.08	784.92	644.29	644.29	28E	438	28a	424
29E	74	0.25	0.13	0.12	0.24	0.05	0.13	0.12	2.69	0.54	0.59	2.93	0.23	0.23	29E	452	29a	438
30E	74	0.25	0.13	0.12	0.24	0.05	0.13	0.12	2.69	0.54	0.59	2.94	0.23	0.23	30E	466	30a	452
31E	74	0.25	0.13	0.12	0.24	0.05	0.13	0.12	2.70	0.54	0.59	2.94	0.24	0.24	31E	480	31a	466
TOTAL			55133.9	52719.98	105440.0	21088.0		4149.23	92205.01	18441.00	39528.99	40714.77	34643.22	34643.22				
6DE	101	0.27	3229.6	2709.92	5419.8	1084.0	0.13	0.11	2.51	0.50	1084.47	116.19	1070.53	1070.53	6de	174	6da	146
7DE	115	0.30	2073.1	1764.31	3528.6	705.7	0.15	0.13	2.82	0.56	706.29	3.07	705.92	705.92	7de	188	7da	160
8DE	129	0.25	3618.5	3116.94	6233.9	1246.8	0.13	0.11	2.40	0.48	1247.26	2.62	1246.94	1246.94	8de	202	8da	174
9DE	185	0.39	10810.0	9408.73	18817.5	3763.5	0.19	0.17	3.74	0.75	3764.24	4.08	3763.75	3763.75	9de	216	9da	188
10DE	199	0.31	349.7	307.08	614.2	122.8	0.16	0.14	3.03	0.61	123.44	3.30	123.04	123.04	10de	230	10da	202
11DE	213	0.44	368.0	325.77	651.5	130.3	0.22	0.19	4.30	0.86	131.17	4.69	130.60	130.60	11de	244	11da	216
12DE	227	0.57	573.0	510.83	1021.7	204.3	0.29	0.26	5.67	1.13	205.47	6.18	204.73	204.73	12de	258	12da	230
13DE	241	0.49	0.24	0.22	0.4	0.09	0.24	0.22	4.84	0.97	1.05	5.27	0.42	0.42	13de	272	13da	244
14DE	255	0.97	0.49	0.44	0.9	0.18	0.49	0.44	9.76	1.95	2.13	10.64	0.85	0.85	14de	286	14da	258
TOTAL			21022.6	18144.24	36288.5	7257.7		1.76	39.06	7.81	7265.51	156.03	7246.78	7246.78				
iph	163	0.10	0.05	0.04	0.09	0.02	0.05	0.04	0.95	0.19	0.21	1.04	0.08	0.08	iph	194	corre.acid	166
ph	163	0.10	2060.5	1763.10	3526.21	705.2	0.05	0.04	0.95	0.19	705.43	45.15	700.01	700.01	ph	194		166
iph	163	0.10	59.2	50.63	101.26	20.3	0.05	0.04	0.95	0.19	20.44	1.04	20.32	20.32	iph	194		166
o-ph	177	0.05	375.0	324.53	649.05	129.8	0.03	0.02	0.46	0.10	129.91	4.40	129.38	129.38	o-ph	208		180
124BE	221	0.05	310.1	258.42	516.83	103.4	0.03	0.02	0.46	0.09	103.46	1.01	103.34	103.34	124be	252		210
123BE	221	0.05	470.9	392.46	784.91	157.0	1.51	1.26	28.02	5.60	162.59	9.03	161.50	161.50	123be	252		210
135BE	221	0.05	0.03	0.02	0.04	0.01	0.03	0.02	0.46	0.09	0.10	1.05	-0.02	0.03	135be	252		210
1245BE	279	0.02	35.4	29.04	58.07	11.6	0.01	0.01	0.18	0.04	11.65	0.20	11.63	11.63	1245be	310		254
12NE	213	0.05	56.9	50.39	100.78	20.2	0.03	0.02	0.49	0.10	20.25	0.54	20.19	20.19	12ne	244		216
TOTAL			3368.2	2868.62	5737.2	1147.4		1.48	32.95	6.59	1154.04	63.45	1146.48	1146.48				
PE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.04	0.05	0.23	0.02	0.02	PE	316	corre.acid	302
SPE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.04	0.05	0.23	0.02	0.02	SPE	316		302
IPE	241	0.08	0.04	0.04	0.08	0.02	0.04	0.04	0.85	0.17	0.19	0.93	0.07	0.07	IPE	316		302
DHE	229	0.02	60.3	57.59	115.17	23.0	5.02	4.80	106.68	21.34	44.37	128.06	29.00	29.00	DHE	314		300
ODE	253	0.06	43.3	41.42	82.83	16.6	0.03	0.03	0.64	0.13	16.69	18.59	14.46	14.46	ODE	328		314
TOTAL			103.6	99.06	198.1	39.8		4.89	108.59	21.72	61.34	148.04	43.58	43.58				
TOTAL ACIDS						29332.8			92383.6	18477.1	48009.9	41082.3	43060.0	43060.1				

* Total volume	10.0 ml	Analysed volume	5.0 ml		
** Sampling area	5.0 m2				%corr./noncorr.
a: Total volume	10.0 ml	Analysed volume	0.45 ml		90
Gravimetric W (mg m⁻³)	NA				

Jolly's Restaurant Outdoor (JRO)
MR 19/01

MONOESTER			Methanol extract				DCM extract				Total	Correction of blanks		Correction with 0.5DL				
name	Ion	DL	E Mass in sample (ng)	A Mass in sample (ng)	Vol correction *	Transfer to ng/m² **	E Mass in sample (ng/450uL)	A Mass in sample (ng/450uL)	Vol correction ^	Transfer to ng/m² **	Total (ng/m²	Total mass in ave FB (ng)	Corrected total (ng/m²)	Corrected total (ng/m²)		Mw		Mw
11E	74	0.10	0.05	0.05	0.09	0.02	0.05	0.05	1.03	0.22	0.23	1.13	-0.12	0.05	11E	200	11a	186
12E	74	0.10	140.1	130.97	261.95	54.57	63.98	59.79	1328.77	276.83	331.40	385.27	211.00	211.00	12E	214	12a	200
13E	74	0.10	0.05	0.05	0.09	0.02	15.44	14.49	322.10	67.10	67.12	1.14	66.77	66.77	13E	228	13a	214
14E	74	0.10	211.7	199.49	396.98	83.12	158.34	149.18	3315.19	690.66	773.79	282.93	691.62	691.62	14E	242	14a	228
15E	74	0.10	101.7	96.11	192.22	40.05	100.74	95.23	2118.29	440.89	480.94	122.10	442.78	442.78	15E	256	15a	242
16E	74	0.15	2261.6	2144.53	4289.06	893.55	1845.87	1750.18	38892.40	8102.58	8996.14	4999.42	7433.82	7433.82	16E	270	16a	256
17E	74	0.10	124.3	118.21	236.42	49.25	96.37	91.62	2036.04	424.18	473.43	363.78	359.75	359.75	17E	284	17a	270
18E	74	0.10	1204.3	1147.77	2295.53	478.24	1122.33	1069.60	23768.91	4951.86	5430.09	3467.77	4340.16	4340.16	18E	298	18a	284
19E	74	0.10	160.7	153.52	307.05	63.97	68.23	65.17	1448.20	301.71	365.68	269.58	275.19	275.19	19E	312	19a	298
20E	74	0.10	1559.4	1491.44	2982.88	621.43	396.27	381.17	8470.45	1764.68	2386.11	3939.69	1154.96	1154.96	20E	326	20a	312
21E	74	0.10	717.3	687.80	1375.59	286.58	171.88	164.81	3662.34	762.99	1049.57	1721.03	511.75	511.75	21E	340	21a	326
22E	74	0.15	4068.6	3926.95	7853.89	1636.23	784.96	753.94	16754.15	3490.45	5126.68	7697.89	2721.09	2721.09	22E	354	22a	340
23E	74	0.10	1845.5	1775.31	3550.62	739.71	353.84	340.18	7559.63	1574.92	2314.64	3186.70	1318.79	1318.79	23E	368	23a	354
24E	74	0.15	8237.8	5045.84	10091.68	2102.43	1165.19	1122.49	24944.12	5196.69	7299.12	8738.25	4568.42	4568.42	24E	382	24a	368
25E	74	0.15	801.5	773.18	1546.37	322.16	202.61	195.45	4343.36	904.87	1227.03	1100.18	883.22	883.22	25E	396	25a	382
26E	74	0.15	2059.6	1969.23	3978.47	828.85	755.03	729.25	16205.53	3376.15	4205.00	3561.97	3065.63	3065.63	26E	410	26a	396
27E	74	0.15	0.06	0.07	0.15	0.03	65.42	63.26	1405.78	292.87	292.90	17.91	287.30	287.30	27E	424	27a	410
28E	74	0.15	429.2	415.47	830.94	173.11	453.72	439.22	9760.49	2033.43	2206.55	784.92	1967.51	1967.51	28E	438	28a	424
29E	74	0.25	0.13	0.12	0.24	0.05	39.60	38.37	852.78	177.66	177.71	2.83	178.79	178.79	29E	452	29a	438
30E	74	0.25	0.13	0.12	0.24	0.05	128.34	124.49	2766.36	576.32	576.38	2.94	575.46	575.46	30E	466	30a	452
31E	74	0.25	0.13	0.12	0.24	0.05	0.13	0.12	2.70	0.56	0.61	2.94	-0.31	0.13	31E	480	31a	466
Total			20943.26	20096.35	40192.7	8373.5				35407.63	43781.11	40670.44	31071.60	31072.19				
DIESTER																		
name	Ion																	
6DE	101	0.27	1217.0	1021.17	2042.3	425.5	69.20	66.07	1290.38	268.83	694.32	78.37	669.83	669.83	6da	174	6da	146
7DE	115	0.30	261.7	239.77	479.5	99.9	82.27	70.01	1555.86	324.14	424.04	3.07	423.06	423.06	7da	188	7da	160
8DE	129	0.25	308.6	265.86	531.7	110.8	209.79	180.71	4015.81	836.63	947.40	2.62	946.58	946.58	8da	202	8da	174
9DE	185	0.39	562.4	489.53	979.1	204.0	806.48	701.92	15596.28	3249.64	3453.61	138.64	3410.29	3410.29	9da	216	9da	188
10DE	199	0.31	0.16	0.14	0.3	0.1	89.40	78.51	1744.74	363.49	363.54	3.30	362.51	362.51	10da	230	10da	202
11DE	213	0.44	0.22	0.19	0.4	0.1	42.96	38.05	845.59	176.16	176.25	4.69	174.78	174.78	11da	244	11da	216
12DE	227	0.57	0.29	0.26	0.5	0.1	45.19	40.29	895.24	186.51	186.62	6.18	184.68	184.68	12da	258	12da	230
13DE	241	0.49	0.24	0.22	0.4	0.1	0.22	0.20	4.36	0.91	1.00	5.27	-0.65	0.24	13da	272	13da	244
14DE	255	0.97	0.49	0.44	0.9	0.2	0.29	0.26	5.74	1.20	1.38	10.64	-1.95	0.49	14da	286	14da	258
Total			2371.2	2017.57	4035.1	840.7	1345.80	1168.02	25958.00	5407.50	6248.15	252.78	6169.18	6172.49				
A.E.																		
name	Ion		Mass in fil															
tph	163	0.10	140.74	120.43	240.85	50.18	9.81	8.22	182.73	38.07	88.25	1.04	87.92	87.92	tph	194	corre.acid	166
ph	163	0.10	1060.54	907.47	1814.94	378.11	30.80	26.35	585.57	121.99	500.11	45.15	486.00	486.00	ph	194		166
iph	163	0.10	178.36	150.91	301.82	62.88	0.00	0.00	0.00	0.00	62.88	1.04	62.55	62.55	iph	194		166
o-ph	177	0.05	163.08	141.13	282.26	58.80	12.61	10.91	242.51	50.52	109.33	4.40	107.95	107.95	o-ph	208		180
124BE	221	0.05	192.11	160.10	320.19	66.71	1.78	1.49	33.00	6.88	73.58	1.01	73.27	73.27	124be	252		210
123BE	221	0.05	196.70	163.91	327.83	68.30	3.13	2.61	58.03	12.09	80.39	9.03	77.56	77.56	123be	252		210
135BE	221	0.05	0.03	0.02	0.04	0.01	1.37	1.31	29.05	6.05	6.06	1.05	5.73	5.73	135be	252		210
1245BE	279	0.02	12.18	9.98	19.96	4.16	0.03	0.02	0.46	0.09	4.25	0.20	4.19	4.19	1245be	310		254
12NE	213	0.05	17.56	15.54	31.06	6.48	2.60	2.30	51.16	10.66	17.13	0.54	16.97	16.97	12ne	244		216
Total			1859.30	1669.49	3339.0	695.6		53.21	1182.50	246.36	941.97	63.45	922.15	926.76				
RESIN E.																		
name	Ion		Mass in fil															
PE	121	0.02	0.01	0.01	0.02	0.00	19.38	18.52	411.60	85.75	85.75	0.23	85.66	85.66	PE	316	corre.acid	302
SPE	121	0.02	0.01	0.01	0.02	0.00	0.03	0.02	0.53	0.11	0.11	0.23	0.04	0.04	SPE	316		302
IPE	241	0.06	0.04	0.04	0.08	0.02	0.00	0.00	0.00	0.00	0.02	0.93	-0.27	0.04	IPE	316		302
DHE	239	0.02	39.80	38.02	78.05	15.84	98.22	93.84	2085.36	434.45	450.30	128.06	410.28	410.28	DHE	314		300
ODE	253	0.06	17.24	16.51	33.02	6.86	27.56	26.39	586.34	122.15	129.03	18.59	123.22	123.22	ODE	328		314
Total			57.10	54.59	109.2	22.7					665.21	148.04	618.95	619.26				
Total acids						9932.5				41061.5	51636.5	41134.7	38781.9	38792.7				

* Total volume	10.0 ml	Analysed volume	5.0 ml		% corr./noncorr.
** Sampling area	4.80 m²				75.1
^ Total volume	10.0 ml	Analysed volume	1.82 ml	4.1340526	
Gravimetric W (mg m⁻³)	92.1				
# Kimwipes:	15				

Downsview Indoor (DWI)
MR 19/01

MONOESTER			Methanol extract				DCM extract				Total	Correction of blanks		Correction with 0.5DL					
name	Ion	DL	E Mass in sample (ng)	A Mass in sample (ng)	Vol correction *	Transfer to ng/m³ **	E Mass in sample (ng/450uL)	A Mass in sample (ng/450uL)	Vol correction *	Transfer to ng/m³ **	Total (ng/m³)	Total mass in ave FB (ng)	Corrected total (ng/m³)	Corrected total (ng/m³)		Mw		Mw
11E	74	0.10	0.05	0.05	0.09	0.01	0.05	0.05	1.03	0.15	0.17	1.13	-0.02	0.05	11E	200	11a	186
12E	74	0.10	135.78	126.88	253.76	37.32	44.66	41.73	927.44	136.39	173.71	226.85	137.01	137.01	12E	214	12a	200
13E	74	0.10	0.05	0.05	0.09	0.01	0.05	0.05	1.04	0.15	0.17	1.14	-0.02	0.05	13E	228	13a	214
14E	74	0.10	120.99	113.99	227.96	33.53	65.21	61.44	1365.31	200.78	234.31	55.78	225.28	225.28	14E	242	14a	228
15E	74	0.10	36.45	34.46	68.91	10.13	27.45	25.95	576.64	84.80	94.93	41.26	88.26	88.26	15E	256	15a	242
16E	74	0.15	956.17	906.59	1813.19	266.64	580.39	550.29	12228.77	1798.35	2064.99	256.54	2023.49	2023.49	16E	270	16a	256
17E	74	0.10	60.05	57.09	114.19	16.79	35.97	34.20	760.02	111.77	128.56	1.15	128.37	128.37	17E	284	17a	270
18E	74	0.10	452.78	431.49	862.96	126.91	382.23	364.27	8094.96	1190.44	1317.34	171.20	1289.65	1289.65	18E	298	18a	284
19E	74	0.10	36.73	35.06	70.17	10.32	22.42	21.42	475.92	69.99	80.31	1.16	80.12	80.12	19E	312	19a	298
20E	74	0.10	370.12	354.23	708.46	104.19	195.89	187.48	4166.27	612.89	716.87	6.81	715.77	715.77	20E	326	20a	312
21E	74	0.10	154.20	147.85	295.69	43.48	92.75	88.93	1976.26	290.83	334.11	77.88	321.51	321.51	21E	340	21a	326
22E	74	0.15	776.59	745.88	1491.76	219.38	472.95	454.25	10094.39	1484.47	1703.85	8.41	1702.49	1702.49	22E	354	22a	340
23E	74	0.10	334.38	321.66	643.32	94.61	229.85	221.11	4913.56	722.58	817.19	1.17	817.00	817.00	23E	368	23a	354
24E	74	0.15	915.80	882.23	1764.47	259.48	793.36	764.29	16984.11	2497.66	2757.14	12.00	2755.20	2755.20	24E	382	24a	368
25E	74	0.15	128.59	124.04	248.08	36.48	149.96	144.65	3214.53	472.73	509.21	1.75	508.92	508.92	25E	396	25a	382
26E	74	0.15	342.50	330.80	661.60	97.29	447.12	431.85	9596.63	1411.27	1508.56	1.75	1508.28	1508.28	26E	410	26a	396
27E	74	0.15	14.82	14.33	28.67	4.22	27.12	26.23	582.79	85.70	89.92	1.76	89.64	89.64	27E	424	27a	410
28E	74	0.15	67.82	65.65	131.30	19.31	142.11	137.57	3057.07	449.57	468.88	1.76	468.59	468.59	28E	438	28a	424
29E	74	0.25	0.13	0.12	0.24	0.04	0.13	0.12	2.69	0.40	0.43	2.93	-0.04	0.13	29E	452	29a	438
30E	74	0.25	0.13	0.12	0.24	0.04	22.52	21.84	485.37	71.38	71.41	2.94	70.94	70.94	30E	466	30a	452
31E	74	0.25	0.13	0.12	0.24	0.04	0.13	0.12	2.70	0.40	0.43	2.94	-0.04	0.13	31E	480	31a	466
Total					9365.4	1380.2				11692.26	13072.49	878.30	12930.41	12930.88				

DIESTER																		
name	Ion																	
6DE	101	0.27	130.62	109.60	219.2	32.2	0.13	0.11	2.51	0.37	32.61	2.73	32.16	32.16	6de	174	6da	146
7DE	115	0.30	0.15	0.13	0.3	0.0	0.15	0.13	2.82	0.41	0.45	3.07	-0.05	0.15	7de	188	7da	160
8DE	129	0.25	143.26	123.40	246.8	36.3	0.13	0.11	2.40	0.35	36.65	2.62	36.22	36.22	8de	202	8da	174
9DE	185	0.39	193.32	168.26	336.5	49.5	0.19	0.17	3.74	0.55	50.04	4.06	49.38	49.38	9de	216	9da	188
10DE	199	0.31	0.16	0.14	0.3	0.0	0.16	0.14	3.03	0.44	0.48	3.30	-0.05	0.16	10de	230	10da	202
11DE	213	0.44	0.22	0.19	0.4	0.1	0.22	0.19	4.30	0.63	0.69	4.69	-0.07	0.22	11de	244	11da	216
12DE	227	0.57	0.29	0.26	0.5	0.1	0.29	0.26	5.67	0.83	0.91	6.18	-0.09	0.29	12de	258	12da	230
13DE	241	0.49	0.24	0.22	0.4	0.1	0.24	0.22	4.84	0.71	0.78	5.27	-0.08	0.24	13de	272	13da	244
14DE	255	0.97	0.49	0.44	0.9	0.1	0.49	0.44	9.76	1.44	1.56	10.64	-0.16	0.49	14de	286	14da	258
Total					805.3	118.4				5.74	124.16	42.58	117.28	119.30				

A.E.																		
name	Ion		Mass in fl															
tph	163	0.10	0.05	0.04	0.09	0.01	0.05	0.04	0.95	0.14	0.15	2.27	-0.21	0.05	tph	194	corre.acid	166
ph	163	0.10	520.54	445.41	890.83	131.00	0.05	0.04	0.95	0.14	131.14	56.95	121.93	121.93	ph	194		166
iph	163	0.10	0.05	0.04	0.09	0.01	0.05	0.04	0.95	0.14	0.15	1.04	-0.02	0.05	iph	194		166
o-ph	177	0.05	27.11	23.46	46.92	6.90	0.03	0.02	0.48	0.07	6.97	7.71	5.72	5.72	o-ph	208		180
124BE	221	0.05	15.91	13.26	26.52	3.90	0.03	0.02	0.48	0.07	3.97	0.51	3.89	3.89	124be	252		210
123BE	221	0.05	20.00	16.66	33.33	4.90	1.87	1.56	34.70	5.10	10.00	0.51	9.92	9.92	123be	252		210
135BE	221	0.05	0.03	0.02	0.04	0.01	0.03	0.02	0.48	0.07	0.07	0.51	-0.01	0.03	135be	252		210
1245BE	279	0.02	1.36	1.12	2.23	0.33	0.01	0.01	0.18	0.03	0.35	0.20	0.32	0.32	1245be	310		254
12NE	213	0.05	0.03	0.02	0.04	0.01	0.03	0.02	0.49	0.07	0.08	0.54	-0.01	0.03	12ne	244		216
Total					1000.1	147.1				5.83	152.90	70.24	141.54	141.94				

RESIN E.																		
name	Ion		Mass in fl															
PE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.03	0.03	0.23	0.00	0.01	PE	316	corre.acid	302
SPE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.03	0.03	0.23	0.00	0.01	SPE	316		302
IPE	241	0.08	0.04	0.04	0.08	0.01	0.04	0.04	0.85	0.12	0.14	0.93	-0.01	0.04	IPE	316		302
DHE	239	0.02	19.83	18.95	37.90	5.57	15.56	14.87	330.43	48.59	54.17	11.10	52.37	52.37	DHE	314		300
ODE	253	0.06	21.74	20.81	41.62	6.12	29.96	28.68	637.38	93.73	99.85	0.70	99.74	99.74	ODE	328		314
Total					79.6	11.7				142.51	154.22	13.19	152.09	152.17				

Total acids						1857.4				11846.4	13503.8	1004.3	13341.3	13344.3				

* Total volume	10.0 ml	Analysed volume	5.0 ml	
** Sampling area	6.80 m^2			%corr/noncorr.
a: Total volume	10.0 ml	Analysed volume	1.75 ml	99
Gravimetric W (mg m^{-2})	NA			
# Kimwipes:	11			

Downsview Outdoor (DWO)
MR 19/01

MONOESTER			Methanol extract				DCM extract				Total	Correction of blanks		Correction with 0.5DL				
name	Ion	DL	E Mass in sample (ng)	A Mass in sample (ng)	Vol correction *	Transfer to ng/m³ **	E Mass in sample (ng/450uL)	A Mass in sample (ng/450uL)	Vol correction *	Transfer to ng/m³ **	Total (ng/m³)	Total mass in avg FB (ng)	Corrected total (ng/m³)	Corrected total (ng/m³)		Mw		Mw
11E	74	0.10	0.05	0.05	0.09	0.01	0.05	0.05	1.03	0.12	0.13	1.13	-0.03	0.05	11E	200	11a	188
12E	74	0.10	82.47	77.07	154.15	17.92	34.94	32.68	725.69	84.38	102.31	305.27	48.55	48.55	12E	214	12a	200
13E	74	0.10	0.05	0.05	0.09	0.01	0.05	0.05	1.04	0.12	0.13	1.14	-0.03	0.05	13E	228	13a	214
14E	74	0.10	235.83	222.00	443.99	51.63	85.72	80.76	1784.84	208.68	260.31	262.93	223.62	223.62	14E	242	14a	228
15E	74	0.10	139.57	131.84	263.67	30.68	75.13	71.02	1578.30	183.52	214.21	122.10	187.17	187.17	15E	256	15a	242
16E	74	0.15	13552.83	12950.09	25700.18	2988.39	4478.26	4247.00	94377.89	10974.17	13962.56	4999.42	13264.97	13264.97	16E	270	16a	256
17E	74	0.10	240.61	228.75	457.51	53.20	69.92	66.47	1477.22	171.77	224.97	363.78	174.21	174.21	17E	284	17a	270
18E	74	0.10	3578.23	3410.12	6820.24	793.05	1068.35	1018.16	22625.71	2630.90	3423.95	3487.77	2937.20	2937.20	18E	298	18a	284
19E	74	0.10	213.95	204.26	408.52	47.50	33.74	32.23	716.23	83.28	130.78	289.58	90.38	90.38	19E	312	19a	298
20E	74	0.10	2557.44	2447.61	4895.22	569.21	303.34	290.32	6451.50	750.17	1319.38	3839.69	769.66	769.66	20E	326	20a	312
21E	74	0.10	1055.03	1011.58	2023.17	235.25	77.90	74.69	1659.89	193.01	428.26	1721.03	188.12	188.12	21E	340	21a	326
22E	74	0.15	5812.52	5582.64	11165.28	1298.29	493.88	474.34	10540.89	1225.70	2523.98	7697.89	1449.86	1449.86	22E	354	22a	340
23E	74	0.10	2540.14	2443.50	4887.00	568.26	189.19	181.78	3595.41	418.07	986.33	3186.70	541.67	541.67	23E	368	23a	354
24E	74	0.15	6809.78	6547.52	12735.03	1480.82	736.06	706.69	15757.45	1832.26	3313.08	8739.25	2093.79	2093.79	24E	382	24a	368
25E	74	0.15	988.14	953.21	1906.41	221.68	123.42	119.06	2645.75	307.65	529.32	1100.18	375.81	375.81	25E	396	25a	382
26E	74	0.15	2692.70	2600.78	5201.52	604.93	665.53	642.80	14264.45	1660.09	2265.81	3581.87	1788.00	1788.00	26E	410	26a	396
27E	74	0.15	189.95	182.72	365.43	42.49	92.02	90.30	1117.79	129.98	172.47	17.91	169.97	169.97	27E	424	27a	410
28E	74	0.15	746.25	722.39	1444.78	168.00	605.32	585.97	13021.57	1514.14	1682.13	784.92	1575.40	1575.40	28E	438	28a	424
29E	74	0.25	89.23	86.46	172.92	20.11	53.06	51.42	1142.58	132.86	152.97	2.83	152.58	152.58	29E	452	29a	438
30E	74	0.25	137.51	133.37	266.75	31.02	224.66	217.91	4842.39	563.07	594.09	2.84	593.68	593.68	30E	466	30a	452
31E	74	0.25	0.13	0.12	0.24	0.03	0.13	0.12	2.70	0.31	0.34	2.84	-0.07	0.13	31E	480	31a	466
Total					79312.4	9222.4				23065.14	32287.51	40670.44	26612.57	26612.91				

DIESTER																		
name	Ion																	
6DE	101	0.27	526.21	441.53	883.1	102.7	0.13	0.11	2.61	0.29	102.97	78.37	92.04	92.04	6de	174	6dn	148
7DE	115	0.30	212.25	180.64	361.3	42.0	61.81	52.60	1188.92	135.92	177.93	3.07	177.50	177.50	7de	188	7dn	160
8DE	129	0.25	800.23	689.31	1378.6	160.3	0.13	0.11	2.49	0.28	160.58	2.82	160.22	160.22	8de	202	8dn	174
9DE	185	0.39	1865.31	1623.51	3247.0	377.6	201.41	175.30	3895.86	452.89	830.55	138.64	811.20	811.20	9de	218	9dn	188
10DE	199	0.31	129.52	113.75	227.5	26.5	43.21	37.95	843.34	98.06	124.52	3.50	124.06	124.06	10de	230	10dn	202
11DE	213	0.44	24.61	21.79	43.6	5.1	0.22	0.19	4.30	0.50	5.57	4.69	4.81	4.81	11de	244	11dn	216
12DE	227	0.57	80.92	72.14	144.3	16.8	0.29	0.26	5.87	0.68	17.44	0.18	16.57	16.57	12de	258	12dn	230
13DE	241	0.49	0.24	0.22	0.4	0.1	0.24	0.22	4.84	0.56	0.61	5.27	-0.12	0.24	13de	272	13dn	244
14DE	255	0.97	0.49	0.44	0.9	0.1	0.49	0.44	9.76	1.14	1.24	10.84	-0.25	0.49	14de	286	14dn	258
Total					6296.7	731.0				690.39	1421.40	252.78	1388.13	1387.23				

A.E.																		
name	Ion		Mass in fil															
tph	163	0.10	126.25	108.03	216.06	25.12	0.05	0.04	0.95	0.11	25.23	1.04	25.08	25.08	tph	194	corre.acid	168
ph	163	0.10	887.13	758.09	1516.18	176.53	20.87	17.89	393.06	45.70	222.24	45.15	215.84	215.84	ph	194		168
bph	163	0.10	107.48	91.87	183.84	21.38	0.05	0.04	0.95	0.11	21.50	1.04	21.35	21.35	bph	194		168
e-ph	177	0.05	189.25	161.77	327.54	38.09	2.00	1.73	38.51	4.48	42.58	4.40	41.95	41.95	e-ph	208		180
124BE	221	0.05	52.90	44.13	88.26	10.26	0.03	0.02	0.48	0.05	10.32	1.01	10.18	10.18	124be	252		210
123BE	221	0.05	123.09	102.58	205.13	23.85	0.03	0.02	0.48	0.05	23.91	0.03	22.65	22.65	123be	252		210
135BE	221	0.05	6.87	5.73	11.46	1.33	0.03	0.02	0.48	0.05	1.38	1.05	1.24	1.24	135be	252		210
1245BE	279	0.02	5.61	4.59	9.18	1.07	0.01	0.01	0.19	0.02	1.09	0.20	1.06	1.06	1245be	310		254
12NE	213	0.05	8.76	7.76	15.51	1.80	0.03	0.02	0.48	0.06	1.86	0.54	1.78	1.78	12ne	244		216
Total					2575.3	299.5				50.64	350.09	63.45	341.24	342.72				

RESIN E.																		
name	Ion		Mass in fil															
PE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.03	0.23	-0.01	0.01	PE	318	corre.acid	302
SPE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.03	0.23	-0.01	0.01	SPE	318		302
IPE	241	0.08	0.04	0.04	0.08	0.01	0.04	0.04	0.85	0.10	0.11	0.93	-0.02	0.04	IPE	318		302
DHE	239	0.02	41.93	40.06	80.13	9.32	67.09	64.84	1212.02	140.93	150.25	128.08	132.38	132.38	DHE	314		300
ODE	253	0.06	18.25	16.43	36.86	4.29	22.43	21.47	477.13	55.48	59.77	18.58	57.17	57.17	ODE	328		314
Total					117.1	13.6				196.56	210.18	148.04	189.52	189.61				

Total acids						19266.4				24002.7	34269.2	41134.7	28529.6	28532.6

* Total volume	10.0 ml	Analysed volume	8.0 ml			%corr./noncorr.
** Sampling area	8.90 m²					83.3
a: Total volume	10.0 ml	Analysed volume	1.93 ml			
Gravimetric W (mg m⁻³)	90.7					
# Rimwipes:	12					

Residential Field Blank Indoor (RSIFB)

MR 19/01

MONOESTER		Methanol extract					DCM extract				MeOH + DCM extract					
name	Ion	Detection limit	E Mass in sample (ng)	A Mass in sample (ng)	Vol correction (ng)*	Transfer to ng/m² **	E Mass in sample (ng/450ul)	A Mass in sample (ng/450ul)	Vol correction *	Transfer to ng/m² **	Total (ng/m²)	Total mass in blank (ng)		Mw		Mw
11E	74	0.10	0.05	0.05	0.09	0.01	0.05	0.05	1.03	0.08	0.09	1.13	11E	200	11a	186
12E	74	0.10	121.56	113.61	227.22	17.35	8.18	7.64	169.88	12.97	30.31	397.10	12E	214	12a	200
13E	74	0.10	0.05	0.05	0.09	0.01	0.05	0.05	1.04	0.08	0.09	1.14	13E	228	13a	214
14E	74	0.10	58.46	55.08	110.16	8.41	8.09	7.62	169.30	12.92	21.33	279.46	14E	242	14a	228
15E	74	0.10	0.05	0.05	0.09	0.01	0.05	0.05	1.05	0.08	0.09	1.14	15E	256	15a	242
16E	74	0.15	136.88	129.76	259.52	19.81	159.37	151.10	3357.65	256.32	276.14	3617.37	16E	270	16a	256
17E	74	0.10	0.05	0.05	0.10	0.01	12.65	12.03	267.35	20.41	20.42	267.45	17E	284	17a	270
18E	74	0.10	74.75	71.24	142.47	10.88	125.34	119.45	2654.44	202.63	213.50	2796.91	18E	298	18a	284
19E	74	0.10	0.05	0.05	0.10	0.01	11.99	11.45	254.55	19.43	19.44	254.65	19E	312	19a	298
20E	74	0.10	0.05	0.05	0.10	0.01	169.15	161.88	3597.40	274.61	274.62	3597.50	20E	326	20a	312
21E	74	0.10	0.05	0.05	0.10	0.01	78.46	75.23	1671.68	127.61	127.62	1671.77	21E	340	21a	326
22E	74	0.15	20.19	19.40	36.79	2.96	365.98	351.50	7811.15	596.27	599.23	7849.95	22E	354	22a	340
23E	74	0.10	0.05	0.05	0.10	0.01	144.39	138.69	3066.51	235.61	235.62	3066.61	23E	368	23a	354
24E	74	0.15	29.81	28.71	57.43	4.38	433.95	416.05	9289.95	709.18	713.54	9347.36	24E	382	24a	368
25E	74	0.15	0.08	0.07	0.14	0.01	66.67	64.31	1429.13	109.09	109.11	1429.28	25E	396	25a	382
26E	74	0.15	23.07	22.28	44.56	3.40	203.42	196.48	4366.12	333.29	336.69	4410.69	26E	410	26a	396
27E	74	0.15	0.08	0.07	0.15	0.01	0.08	0.07	1.61	0.12	0.13	1.76	27E	424	27a	410
28E	74	0.15	0.08	0.07	0.15	0.01	49.88	48.28	1072.97	81.91	81.92	1073.11	28E	438	28a	424
29E	74	0.25	0.13	0.12	0.24	0.02	0.13	0.12	2.69	0.21	0.22	2.93	29E	452	29a	438
30E	74	0.25	0.13	0.12	0.24	0.02	0.13	0.12	2.69	0.21	0.22	2.94	30E	466	30a	452
31E	74	0.25	0.13	0.12	0.24	0.02	0.13	0.12	2.70	0.21	0.22	2.94	31E	480	31a	466
Total					882.1	67.3			39211.10	2993.21	3060.55	40093.18				
DIESTER																
name	Ion															
6DE	101	0.27	50.44	42.33	84.7	6.5	0.13	0.11	2.51	0.19	6.65	87.16	6de	174	6da	146
7DE	115	0.30	0.15	0.13	0.3	0.0	0.15	0.13	2.62	0.22	0.23	3.07	7de	188	7da	160
8DE	129	0.25	0.13	0.11	0.2	0.0	0.13	0.11	2.40	0.18	0.20	2.62	8de	202	8da	174
9DE	185	0.39	0.19	0.17	0.3	0.0	0.19	0.17	3.74	0.29	0.31	4.08	9de	216	9da	188
10DE	199	0.31	0.16	0.14	0.3	0.0	0.16	0.14	3.03	0.23	0.25	3.30	10de	230	10da	202
11DE	213	0.44	0.22	0.19	0.4	0.0	0.22	0.19	4.30	0.33	0.36	4.69	11de	244	11da	216
12DE	227	0.57	0.29	0.26	0.5	0.0	0.29	0.26	5.67	0.43	0.47	6.18	12de	258	12da	230
13DE	241	0.49	0.24	0.22	0.4	0.0	0.24	0.22	4.84	0.37	0.40	5.27	13de	272	13da	244
14DE	255	0.97	0.49	0.44	0.9	0.1	0.49	0.44	9.76	0.75	0.81	10.64	14de	286	14da	258
Total					87.9	6.7			39.06	2.98	9.69	127.00				
A.E.																
name	Ion		Mass in fil													
iph	163	0.10	0.05	0.04	0.09	0.01	0.05	0.04	0.95	0.07	0.08	1.04	iph	194	corre.acid	166
ph	163	0.10	20.96	17.93	35.86	2.74	0.05	0.04	0.95	0.07	2.81	36.81	ph	194		166
iph	163	0.10	0.05	0.04	0.09	0.01	0.05	0.04	0.95	0.07	0.08	1.04	iph	194		166
o-ph	177	0.05	0.03	0.02	0.04	0.00	0.03	0.02	0.48	0.04	0.04	0.52	o-ph	208		180
124BE	221	0.05	0.03	0.02	0.04	0.00	0.03	0.02	0.48	0.04	0.04	0.50	124be	252		210
123BE	221	0.05	0.03	0.02	0.04	0.00	0.03	0.02	0.48	0.04	0.04	0.50	123be	252		210
135BE	221	0.05	0.03	0.02	0.04	0.00	0.03	0.02	0.48	0.04	0.04	0.50	135be	252		210
1245BE	279	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.18	0.01	0.02	0.20	1245be	310		254
12NE	213	0.05	0.03	0.02	0.04	0.00	0.03	0.02	0.49	0.04	0.04	0.54	12ne	244		216
Total					36.3	2.8			5.40	0.41	3.18	41.66				
RESIN E.																
name	Ion		Mass in fil													
PE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.02	0.23	PE	316	corre.acid	302
SPE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.02	0.23	SPE	316		302
IPE	241	0.08	0.04	0.04	0.08	0.01	0.04	0.04	0.85	0.06	0.07	0.93	IPE	316		302
DHE	239	0.02	8.56	8.18	16.35	1.25	4.21	4.02	89.43	6.83	8.08	105.78	DHE	314		300
ODE	253	0.06	0.03	0.03	0.06	0.00	0.03	0.03	0.64	0.05	0.05	0.70	ODE	328		314
Total					16.5	1.3			91.34	6.97	8.23	107.87				
Total acids					1022.8	78.1			39346.9	3003.6	3081.7	40369.7				

* Total volume 10.0 ml Analysed volume 5.0 ml

** Sampling area 13.10 m² (the same area as residential indoor sample)

a: Total volume 10.0 ml Analysed volume 1.65 ml

Jolly's Restaurant Field Blank Outdoor (JROFB)

MR 19/01

MONOESTER		Methanol extract					DCM extract				MeOH + DCM extract						
name	Ion	Detection limit	E Mass in sample (ng)	A Mass in sample (ng)	Vol correction (ng)*	Transfer to ng/m2 **	E Mass in sample (ng/450ul)	A Mass in sample (ng/450ul)	Vol correction *	Transfer to ng/m² **	Total (ng/m²)	Total mass in blank (ng)		Mw		Mw
11E	74	0.10	0.05	0.05	0.09	0.01	0.05	0.05	1.03	0.12	0.13	1.13	11E	200	11a	186
12E	74	0.10	69.62	65.07	130.13	15.13	14.79	13.82	307.06	35.71	50.84	437.19	12E	214	12a	200
13E	74	0.10	0.05	0.05	0.09	0.01	0.05	0.05	1.04	0.12	0.13	1.14	13E	228	13a	214
14E	74	0.10	61.41	57.86	115.71	13.46	10.30	9.70	215.65	25.06	38.53	331.37	14E	242	14a	228
15E	74	0.10	47.95	45.33	90.66	10.54	6.20	5.86	130.26	15.15	25.69	220.92	15E	256	15a	242
16E	74	0.15	1127.53	1069.07	2136.13	248.62	190.23	180.36	4006.04	466.05	714.67	6146.17	16E	270	16a	256
17E	74	0.10	65.79	62.55	125.09	14.55	13.68	13.00	288.94	33.60	48.14	414.03	17E	284	17a	270
18E	74	0.10	661.83	649.80	1299.60	151.12	108.24	103.15	2292.28	266.54	417.66	3591.67	18E	298	18a	284
19E	74	0.10	85.75	82.80	125.60	14.60	9.22	8.81	195.69	22.76	37.36	321.29	19E	312	19a	298
20E	74	0.10	881.80	843.93	1687.86	196.26	132.74	127.04	2823.20	328.28	524.54	4511.06	20E	326	20a	312
21E	74	0.10	314.22	301.28	602.56	70.07	54.79	52.54	1167.52	135.76	205.82	1770.08	21E	340	21a	326
22E	74	0.15	1186.21	1139.30	2278.60	264.95	268.61	257.99	5733.00	666.63	931.58	8011.60	22E	354	22a	340
23E	74	0.10	398.56	383.40	766.79	89.16	123.58	118.88	2641.70	307.17	396.34	3408.50	23E	368	23a	354
24E	74	0.15	824.37	794.18	1588.31	184.69	329.82	317.73	7060.77	821.02	1005.71	8649.09	24E	382	24a	368
25E	74	0.15	101.35	97.77	195.53	22.74	21.99	21.22	471.48	54.82	77.56	667.01	25E	396	25a	382
26E	74	0.15	256.35	247.60	495.19	57.58	123.88	119.65	2656.99	309.18	366.77	3154.18	26E	410	26a	396
27E	74	0.15	0.08	0.07	0.15	0.02	0.08	0.07	1.61	0.19	0.20	1.76	27E	424	27a	410
28E	74	0.15	32.33	31.30	62.59	7.28	24.42	23.64	525.33	61.08	68.36	587.92	28E	438	28a	424
29E	74	0.25	0.13	0.12	0.24	0.03	0.13	0.12	2.69	0.31	0.34	2.93	29E	452	29a	438
30E	74	0.25	0.13	0.12	0.24	0.03	0.13	0.12	2.69	0.31	0.34	2.94	30E	466	30a	452
31E	74	0.25	0.13	0.12	0.24	0.03	0.13	0.12	2.70	0.31	0.34	2.94	31E	480	31a	466
Total					11703.4	1360.9				3550.20	4911.06	42235.11				
DIESTER																
name	Ion															
6DE	101	0.27	85.04	71.36	142.7	16.6	0.13	0.11	2.51	0.29	16.89	145.22	6de	174	6da	146
7DE	115	0.30	0.15	0.13	0.3	0.0	0.15	0.13	2.82	0.33	0.36	3.07	7de	188	7da	160
8DE	129	0.25	0.13	0.11	0.2	0.0	0.13	0.11	2.40	0.28	0.30	2.62	8de	202	8da	174
9DE	185	0.39	0.18	0.17	0.3	0.0	0.19	0.17	3.74	0.43	0.47	4.08	9de	216	9da	188
10DE	199	0.31	0.16	0.14	0.3	0.0	0.16	0.14	3.03	0.35	0.38	3.30	10de	230	10da	202
11DE	213	0.44	0.22	0.19	0.4	0.0	0.22	0.19	4.30	0.50	0.54	4.69	11de	244	11da	216
12DE	227	0.57	0.29	0.26	0.5	0.1	0.29	0.26	5.67	0.66	0.72	6.18	12de	258	12da	230
13DE	241	0.49	0.24	0.22	0.4	0.1	0.24	0.22	4.84	0.56	0.61	5.27	13de	272	13da	244
14DE	255	0.97	0.49	0.44	0.9	0.1	0.49	0.44	9.76	1.14	1.24	10.64	14de	286	14da	258
Total					146.0	17.0				4.54	21.52	185.06				
A.E.																
name	Ion		Mass in fil													
iph	163	0.10	0.05	0.04	0.09	0.01	0.05	0.04	0.95	0.11	0.12	1.04	iph	194	corre.acid	166
ph	163	0.10	12.14	10.39	20.78	2.42	0.05	0.04	0.95	0.11	2.53	21.73	ph	194		166
iph	163	0.10	0.05	0.04	0.09	0.01	0.05	0.04	0.95	0.11	0.12	1.04	iph	194		166
o-ph	177	0.05	6.74	5.83	11.67	1.36	0.03	0.02	0.48	0.06	1.41	12.15	o-ph	208		180
124BE	221	0.05	0.93	0.78	1.55	0.18	0.03	0.02	0.46	0.05	0.23	2.01	124be	252		210
123BE	221	0.05	3.73	3.11	6.22	0.72	0.03	0.02	0.46	0.05	0.78	6.68	123be	252		210
135BE	221	0.05	1.00	0.83	1.67	0.19	0.03	0.02	0.46	0.05	0.25	2.13	135be	252		210
1245BE	279	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.18	0.02	0.02	0.20	1245be	310		254
12NE	213	0.05	0.03	0.02	0.04	0.01	0.03	0.02	0.49	0.06	0.06	0.54	12ne	244		216
Total					42.1	4.9				0.63	5.52	47.50				
RESIN E.																
name	Ion		Mass in fil													
PE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.03	0.23	PE	316	corre.acid	302
SPE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.03	0.23	SPE	316		302
IPE	241	0.08	0.04	0.04	0.08	0.01	0.04	0.04	0.85	0.10	0.11	0.93	IPE	316		302
DHE	239	0.02	26.29	25.12	50.24	5.84	5.29	5.06	112.39	13.07	18.91	162.63	DHE	314		300
ODE	253	0.06	14.66	14.03	28.07	3.26	0.03	0.03	0.64	0.07	3.34	28.71	ODE	328		314
Total					78.4	9.1				13.29	22.41	192.72				
Total acids						1391.9				3568.7	4960.5	42660.4				

* Total volume 10.0 ml Analysed volume 5.0 ml

** Sampling area 8.60 m² (the same as outdoor sample area)

a: Total volume 10.0 ml Analysed volume 1.75 ml

Egbert Field Blank Outdoor (EBOFB)

MR 26/01

MONOESTER			Methanol extract				DCM extract				MeOH + DCM extract							
name	Ion	Detection limit	E Mass in sample (ng)	A Mass in sample (ng)	Vol correction (ng)*	Transfer to ng/m² **	E Mass in sample (ng/450ul)	A Mass in sample (ng/450ul)	Vol correction *	Transfer to ng/m² **	Total (ng/m²)	Total mass in blank (ng)		Mw		Mw
11E	74	0.10	0.05	0.05	0.09	0.01	0.05	0.05	1.03	0.09	0.09	1.13	11E	200	11a	186
12E	74	0.10	171.46	150.25	320.49	26.57	0.05	0.05	1.04	0.09	26.66	321.53	12E	214	12a	200
13E	74	0.10	0.05	0.05	0.09	0.01	0.05	0.05	1.04	0.09	0.09	1.14	13E	228	13a	214
14E	74	0.10	93.89	88.45	176.91	14.67	0.05	0.05	1.05	0.09	14.76	177.96	14E	242	14a	228
15E	74	0.10	75.74	71.59	143.19	11.87	0.05	0.05	1.05	0.09	11.96	144.24	15E	256	15a	242
16E	74	0.15	1378.18	1306.72	2613.43	216.70	124.41	117.96	2621.29	217.35	434.06	5234.72	16E	270	16a	256
17E	74	0.10	115.31	109.62	218.25	18.18	9.02	8.58	190.62	15.81	33.99	409.87	17E	284	17a	270
18E	74	0.10	1372.30	1260.17	2520.35	208.96	73.39	69.94	1554.18	128.87	337.85	4074.52	18E	298	18a	284
19E	74	0.10	72.68	69.42	138.84	11.51	7.25	6.92	153.89	12.76	24.27	292.73	19E	312	19a	298
20E	74	0.10	1064.05	1018.35	2036.71	168.88	78.70	75.32	1673.79	138.79	307.67	3710.50	20E	326	20a	312
21E	74	0.10	432.07	414.28	828.56	68.70	41.90	40.17	892.68	74.02	142.72	1721.24	21E	340	21a	326
22E	74	0.15	2048.89	1967.86	3935.73	326.35	154.45	148.34	3296.39	273.33	599.68	7232.11	22E	354	22a	340
23E	74	0.10	848.62	816.33	1632.67	135.38	67.00	64.45	1432.31	118.77	254.14	3064.96	23E	368	23a	354
24E	74	0.15	2179.18	2099.32	4198.63	348.15	167.77	160.88	4019.65	333.30	681.45	8218.26	24E	382	24a	368
25E	74	0.15	332.00	320.27	640.53	53.11	26.30	25.37	563.73	46.74	99.86	1204.26	25E	396	25a	382
26E	74	0.15	824.91	796.74	1593.48	132.13	73.97	71.44	1567.58	131.64	263.77	3181.06	26E	410	26a	396
27E	74	0.15	25.13	24.30	48.60	4.03	0.08	0.07	1.61	0.13	4.16	50.21	27E	424	27a	410
28E	74	0.15	175.57	169.95	339.91	28.18	13.66	13.22	293.61	24.36	52.55	633.72	28E	438	28a	424
29E	74	0.25	0.13	0.12	0.24	0.02	0.13	0.12	2.69	0.22	0.24	2.93	29E	452	29a	438
30E	74	0.25	0.13	0.12	0.24	0.02	0.13	0.12	2.69	0.22	0.24	2.94	30E	466	30a	452
31E	74	0.25	0.13	0.12	0.24	0.02	0.13	0.12	2.70	0.22	0.24	2.94	31E	480	31a	466
Total					21368.2	1773.5			18294.83	1516.98	3290.47	39663.02				
DIESTER																
name	Ion															
6DE	101	0.27	0.13	0.11	0.2	0.0	0.13	0.11	2.51	0.21	0.23	2.73	6de	174	6da	146
7DE	115	0.30	0.15	0.13	0.3	0.0	0.15	0.13	2.82	0.23	0.25	3.07	7de	188	7da	160
8DE	129	0.25	0.13	0.11	0.2	0.0	0.13	0.11	2.40	0.20	0.22	2.62	8de	202	8da	174
9DE	185	0.39	232.10	202.01	404.0	33.5	0.19	0.17	3.74	0.31	33.81	407.76	9de	216	9da	188
10DE	199	0.31	0.16	0.14	0.3	0.0	0.16	0.14	3.03	0.25	0.27	3.30	10de	230	10da	202
11DE	213	0.44	0.22	0.19	0.4	0.0	0.22	0.19	4.30	0.36	0.39	4.69	11de	244	11da	216
12DE	227	0.57	0.29	0.26	0.5	0.0	0.29	0.26	5.57	0.47	0.51	6.18	12de	258	12da	230
13DE	241	0.49	0.24	0.22	0.4	0.0	0.24	0.22	4.84	0.40	0.44	5.27	13de	272	13da	244
14DE	255	0.97	0.49	0.44	0.9	0.1	0.49	0.44	9.76	0.81	0.88	10.64	14de	286	14da	258
Total					407.2	33.8			39.06	3.24	37.00	446.26				
A.E.																
name	Ion		Mass in fil													
tph	163	0.10	0.05	0.04	0.09	0.01	0.05	0.04	0.95	0.08	0.09	1.04	tph	194	corre.acid	166
ph	163	0.10	44.39	37.99	75.97	6.30	0.05	0.04	0.95	0.08	6.38	76.92	ph	194		166
tph	163	0.10	0.05	0.04	0.09	0.01	0.05	0.04	0.95	0.08	0.09	1.04	tph	194		166
o-ph	177	0.05	0.03	0.02	0.04	0.00	0.03	0.02	0.48	0.04	0.04	0.52	o-ph	208		180
124BE	221	0.05	0.03	0.02	0.04	0.00	0.03	0.02	0.46	0.04	0.04	0.50	124be	252		210
123BE	221	0.05	11.67	9.73	19.45	1.61	0.03	0.02	0.46	0.04	1.65	19.91	123be	252		210
135BE	221	0.05	0.03	0.02	0.04	0.00	0.03	0.02	0.46	0.04	0.04	0.50	135be	252		210
1245BE	279	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.18	0.02	0.02	0.20	1245be	310		254
12NE	213	0.05	0.03	0.02	0.04	0.00	0.03	0.02	0.49	0.04	0.04	0.54	12ne	244		216
Total					95.8	7.9			5.40	0.45	8.39	101.16				
RESIN E.																
name	Ion		Mass in fil													
PE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.02	0.23	PE	316	corre.acid	302
SPE	121	0.02	0.01	0.01	0.02	0.00	0.01	0.01	0.21	0.02	0.02	0.23	SPE	316		302
IPE	241	0.08	0.04	0.04	0.08	0.01	0.04	0.04	0.85	0.07	0.08	0.93	IPE	316		302
DHE	229	0.02	14.59	13.84	27.87	2.31	4.14	3.96	87.90	7.29	9.60	115.77	DHE	314		300
ODE	253	0.06	13.66	13.06	26.16	2.17	0.01	0.01	0.21	0.02	2.19	28.37	ODE	328		314
Total					54.1	4.5			89.38	7.41	11.90	143.53				
Total acids					21945.3	1819.7			18428.7	1528.1	3347.8	40374.0				

* Total volume 10.0 ml Analysed volume 5.0 ml

** Sampling area 12.06 m²

a: Total volume 10.0 ml Analysed volume 1.57 ml