

"Four stages of acceptance:

- i) this is worthless nonsense,
- ii) this is an interesting, but perverse, point of view,
- iii) this is true, but quite unimportant,
- iv) I always said so."

-J.B.S. Haldane (1892-1964), English geneticist

University of Alberta

Predicting the age of weathered hydrocarbon mixtures

by

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Abstract

Predicting the time for which a petroleum mixture has been exposed to weathering effects could have many applications. Historically, research on the evaporation rates of hydrocarbon mixtures has focused on forensic oil spill identification. Relatively little attention has focused on estimating the exposure time for a weathered petroleum sample based on the observed composition at a given time, and assuming a prior composition.

A hierarchical application of multivariate techniques was used to estimate the time for which a hydrocarbon mixture was exposed to evaporative weathering. Partial least squares discriminant analysis (PLS-DA) could predict whether a sample was relatively fresh (< 12 hours exposure time) or highly weathered (> 20 hours exposure time). Subsequent regression models for these classes were evaluated for accuracy using the root mean square error of prediction (RMSEP). One nonlinear regression model in particular was found to satisfactorily estimate the age of weathered petroleum samples.

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List of Symbols

$[A]_m$ – Equilibrium concentration of analyte in the mobile phase

$[A]_s$ – Equilibrium concentration of analyte in the stationary phase

α – Selectivity factor; weighting parameter in generalized least squares weighting

β – Phase ratio

\mathbf{C} – Covariance matrix

C_s – Concentration of analyte in stationary phase

C_m – Concentration of analyte in the mobile phase

\mathbf{D} – Weighted and ridged version of the singular values matrix

d_c – Inner diameter of the column

d_f – Film thickness

\mathbf{G} – Filtering matrix in generalized least squares weighting

I_d – Identity matrix

K_c – Distribution coefficient

k – Retention factor

m – Number of elements in a matrix

N – Number of theoretical plates

n – Peak capacity; the number of samples in a test set

r_c – Radius of the column

R_s – Resolution

\mathbf{S} – Diagonal matrix of singular values

s_{yd} – Standard deviation of y-value differences

t_m – Dead-time or hold-up time

t_r – Retention time

t_{r_max} – Maximum retention time of a system

\mathbf{V} – Matrix of eigenvectors

V_M – Mobile phase volume

V_S – Stationary phase volume

\mathbf{W} – Re-weighting matrix

w_b – Peak width at the baseline

w_i – Diagonal element in the re-weighting matrix

\mathbf{X}_d – Matrix of derivatives for the X-block

\mathbf{y}_d – Matrix of y-block derivatives

$\mathbf{y}_{d,i}$ – The i^{th} element of the \mathbf{y}_d vector

$\bar{\mathbf{y}}_d$ – Average of elements in vector \mathbf{y}_d

y_i – true y-value of the sample i

\hat{y}_i – y-value predicted for sample i with the model under evaluation

List of Abbreviations

ANN – Artificial neural networks

BTEX – Benzene, toluene, ethylbenzene and xylenes

FID – Flame ionization detector

FT-ICR – Fourier transform ion cyclotron resonance

GC – Gas chromatography

GLSW – Generalized least squares weighting

GRAM – Generalized rank annihilation method

GCxGC – Comprehensive two-dimensional gas chromatography

IL – Ignitable liquid

IR – Infrared (spectroscopy)

IS – Internal standard

LV – Latent variable

LC – Liquid chromatography

LWR – Locally weighted regression

LMCS – Longitudinally modulated cryogenic system

MS – Mass spectrometer/ spectrometry

MTBE – Methyl tert-butyl ether

μ ECD – Micro-electron capture detector

MLR – Multiple linear regression

PolyPLS – Nonlinear PLS regression

PARAFAC – Parallel factor analysis

PLS – Partial least squares

PLS-DA – Partial least squares discriminant analysis

PCA – Principal component analysis

RMSEP – Root mean square error of prediction

SIMCA – Soft independent modelling of class analogy

TOF – Time of flight

UCM – Unresolved complex mixture

WCOT– Wall coated open tubular column

1. Introduction

1.1 Thesis Overview

Petroleum released into the environment is subjected to numerous degradation processes, known collectively as weathering. Understanding the compositional changes that occur during the weathering of a hydrocarbon mixture can aid in evaluating its impact on an ecosystem, making accurate risk assessments and evaluation of remediation strategies. Historically, research on the evaporation rates of petroleum mixtures has focused on forensic oil spill identification and predicting if a fresh sample could be weathered to give an observed composition in an aged sample [1, 2]. Relatively little attention has been focused on approaching the problem from the other direction: estimating the time of exposure based on the observed composition of a weathered sample at a given time, and assuming a prior composition. A few predictive weathering studies of heavier hydrocarbon mixtures have been reported and have proven important in litigation [3, 4]. However, predicting the exposure time of a lighter petroleum mixture such as gasoline has remained relatively unexplored. Predictive models that could estimate the exposure time of a weathered light petroleum sample could have numerous applications, such as aiding forensic investigators establish the cause and intent of a fire.

This thesis describes the application of multivariate techniques to both one-dimensional and comprehensive two-dimensional gas chromatographic (GC×GC) data for the purpose of estimating the age of weathered light petroleum mixtures. Since its inception, GC×GC has been used by the petroleum industry because its large peak capacity and good sensitivity make it an ideal technique for the study of complex samples [5]. Furthermore, chemometric techniques have been successful in elucidating patterns and trends from complex data; specifically data arising from GC×GC and multidimensional analyses in areas such as fragrances [6], wines [7] and food additives [8], as well as petroleum [References 43-54, 78, 80-85].

The first chapter of this thesis reviews the literature pertaining to the weathering and fingerprinting of petroleum mixtures and provides an overview of chemometric techniques and GC×GC. In Chapter 2, the evaluation of a weathering chamber is presented along with a proof-of-concept study using a model hydrocarbon mixture monitored over time by gas chromatography (GC). Weathering patterns were explored using a variety of chemometric models, including partial least squares (PLS), nonlinear PLS (PolyPLS) and locally weighted regression (LWR). Chapter 3 describes weathering studies performed on 87- and 89-octane gasolines using GC×GC analysis and the hierarchical application of chemometric models to predict the age of a weathered sample. A final chapter presents some overall conclusions and recommendations for further study.

1.2 Petroleum weathering

1.2.1 *Hydrocarbon pollution*

Hydrocarbon pollution causing environmental damage occurs frequently due to accidental and intentional release from sources such as production platforms, tanker accidents, operational discharges, municipal waste or natural seepage. Petroleum input into the marine environment has previously been estimated at 1.7-8.8 million metric tons per year [9]. The ability to characterize and observe petroleum spill behaviour is important in evaluating its impact on an ecosystem, making accurate risk assessments, and determining the efficacy of remediation strategies implemented to mitigate damage.

Petroleum released into the environment is subjected to weathering, which encompasses the physical, chemical and biological processes responsible for hydrocarbon degradation. Extensive research has been conducted to improve our understanding of the compositional changes that occur during heavy petroleum weathering, which is essential to determining the fate and behaviour of oil spills in the environment [10, 11]. Stiver and Mackay [12] attempted to quantify the evaporation rate of petroleum mixtures through equations derived from mass transfer theory; later Kawamura and McKay [13] looked at the efficacy of two models developed to estimate the evaporation rates of volatiles resulting from ground spills. Wang and Fingas [14] studied the changes in chemical composition of light crude oil with gas chromatography-mass

spectrometry (GC-MS) and GC with flame ionization detection (GC-FID), then derived mathematical equations to estimate the extent of evaporation in oil. Schoenmakers et al. [15] compared comprehensive GC×GC to GC-MS for the characterization of hydrocarbon mixtures, while Beens and Tijssen [16] applied liquid chromatography coupled to gas chromatography (LC-GC) for the characterization of middle distillate oil fractions. Nelson et al. [17] investigated the weathering of a 2003 fuel oil spill using GC×GC to identify weathering patterns and measure the changes of individual analytes; similarly, Wardlaw et al. [18] used GC×GC for an environmental fate study on natural oil seeps, investigating the compositional changes in petroleum during subsurface degradation.

Previous studies have also focused on the weathering of heavy petroleum samples in more extreme environments. For example, Brandvic and Faksness [19] studied Arctic oil spills and the effect of ice conditions on oil weathering, Barakat et al. [20] investigated biomarker stability in oil exposed to the arid terrestrial environment of Egypt, and Wang et al. [21] collected data on a 25-year-old oil spill in the wetlands of northern Alberta to determine if clean-up was successful and to assess vegetative recovery. Toxicity during weathering has also been studied to understand the consequences of oil spills for marine ecosystems. Neff et al. [22] studied the toxicity of crude oil and diesel fuel weathering on six tropical and temperate marine animals. Similarly, Carls et

al. [23] have studied crude oil toxicity on pacific herring eggs, and Heintz et al. [24] on pink salmon embryos.

Liability associated with petroleum release in the environment requires reliable characterization and source identification, which can be complicated by weathering. However, understanding this process can aid in determining which criteria are necessary for characterization. Biomarkers are distinctive compounds found in crude oil that are resistant to degradation, making them ideal for predicting efficiency of remedial action, monitoring spill behaviour and identifying oil sources. Consequently, biomarkers have become the focus of many petroleum weathering studies [25]. For example, Fernández-Varela et al. [26] performed a comparative study to evaluate the capabilities of infrared spectroscopy (IR), GC-FID and GC-MS to differentiate fuel oils. Similarly, Wang et al. [27, 28,29] specifically looked at GC-MS to identify and quantify target compounds in a number of petroleum products for source identification, as well as publishing a review of hydrocarbon fingerprinting and identification techniques [30].

Gaines and Frysinger [31] published the first application of GC×GC to oil spill source identification and successfully matched a marine diesel fuel spill to one of two potential sources; they then assessed the ability of GC×GC-MS (quadrupole) to analyze marine diesel fuel for compound identification [32]. These authors also studied the unresolved complex mixture (UCM) in

petroleum-containing sediment using GC×GC [33]. GC×GC analysis of petroleum has also been researched by Vendeuvre et al. [34, 35, 36], while Bertoncini et al. [37] reviewed the applications of multidimensional GC for trace analysis in the petroleum industry. Most recently, Juyal et al. [38] characterized an unusual blue crude oil using GC×GC, Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR-MS), and fluorescence spectroscopy. Van Stee et al. [39] applied GC×GC with atomic emission detection to fingerprint and identify nitrogen and sulphur containing compounds in petroleum, followed by correlation with GC×GC coupled to a time-of-flight mass spectrometer (TOFMS). Some non-chromatographic methods recently used for petroleum fingerprinting include electrospray ionization-mass spectrometry (no fragmentation) [40, 41] and fluorescence spectroscopy [42].

Chemometrics are often applied to interpret petroleum fingerprinting data. Van Mispelaar et al. [43] applied multivariate techniques to GC×GC data for the discrimination of crude oils from different reservoirs within a single oil field. Mudge [44] was able to reassess the sources of hydrocarbon background found in the Gulf of Alaska and Prince William Sound with PLS analysis, while Stout et al. [45] studied petroleum biomarkers using principal component analysis (PCA) to correlate spilled oil to possible sources. Gaines et al. [46] reduced the number of biomarker ratios needed to differentiate between diesel fuels using PCA, while Malmquist et al. [47] distinguished between the effects of evaporation and dissolution on oil spill composition. Pérez-Caballero et al. [48]

studied IR spectroscopy and PCA analysis to identify and monitor hydrocarbon spills in a marine environment, and Borges et al. [49] compared PCA, Kohonen self-organizing maps and partial least squares discriminant analysis (PLS-DA) for the classification of oil samples by geographical origin. Similarly, parallel factor analysis (PARAFAC) has been applied as a screening technique for source matching [50], and soft independent modelling of class analogy (SIMCA) has successfully classified heavy petroleum based on biomarker data [51, 52, 53]. A detailed review has recently been published on oil spill fingerprinting using chemometric techniques [54].

Unfortunately, few studies have focused on light petroleum weathering with the aim to estimate the time of exposure based on the observed composition of a weathered sample at a given time, and assuming a prior composition. Previous studies aimed at estimating the age of petroleum contamination have already proven important in litigation due to the high costs associated with spill clean-up. Oukijk [55] successfully estimated the age of heating-oil leaks from underground storage tanks with an error of ± 2 years. Similarly, Christensen and Larsen [56] studied degradation ratios between alkanes and isoprenoids from which they could estimate the age of diesel oil spills in a subsurface soil environment with an error of ± 2 years for oil exposed between 5-20 years.

1.2.2 Arson Investigation

Another area of interest for petroleum weathering is arson investigation. In the United States, annual property damage from intentional fires is estimated at over one billion dollars [57]. As forensic investigators seek to determine the cause of a fire, identifying the presence of an ignitable liquid (IL) is the primary question, though it is desirable to identify the class and origin of the IL as well. This has led to studies focused on tracing the origin of an IL [58, 59, 60]. Hirz and Rizz [61] developed a method for simulating gasoline weathering through semi-empirical equations which correlate the weathered sample with its original composition, aiding to trace back the weathered sample to the original unweathered source. Mann [62] was successful in using GC to distinguish between unweathered gasolines from different distributors and between gasolines from the same distributor after successive deliveries. A few years later, Jayatilaka and Poole [63] used heartcut GC to separate target compounds from fire debris interference for the identification of ILs.

Traditionally, forensic investigators use GC-MS to identify accelerant in fire debris analysis [64, 65, 66]. However, studies have also expanded into other methods of IL analysis. Fryinger and Gaines [67] identified and classified ILs in fire debris using GC×GC. They have also quantitated BTEX (benzene-toluene-ethylbenzene-xylenes) and total aromatics in gasoline [68] using GC×GC, as well as oxygenates such as C1-C4 alcohols and methyl tert-butyl

ether (MTBE) [69]. Van Deursen et al. [70] analysed kerosene using GC×GC-TOFMS to identify sulphur and oxygen containing compounds, while Hua et al. [71] used GC×GC with a sulphur chemiluminescence detector to ascertain the sulphur containing compounds in diesel oil. DeVos [72] was successful in reducing sample matrix problems from pyrolysis products using GC-MS-MS for the detection of gasoline in fire debris. Similarly, Lu and Harrington [73] investigated gas chromatography-differential mobility spectrometry for identification of ILs in fire debris, while Rodgers et al. [74] used FT-ICR-MS. Alexander et al. [75], as well as Sheff and Siegel [76], studied three-dimensional fluorescence plots for gasoline source identification; this technique was first used in the forensic analysis of motor oils. Studies have also taken an interest in identifying biodiesel fuels and alternative fuel blends from fire debris [77] in order to keep abreast of changes in consumer activity. Pierce and Schale [78] looked at one- and two-dimensional GC-MS, along with PLS to construct models which predict the percent composition of biodiesel in biodiesel blends. Similarly, Seeley et al. [79] used GC×GC to determine the concentration of alcohol in biodiesel blends.

Multivariate analysis is a large area of study currently being applied to the analysis of ILs. Fraga et al. [80] separated aromatic isomers in jet fuel with a GC×GC high-speed quantitative analysis, applying generalized rank annihilation method (GRAM) to resolve the overlapping peaks. Petraco et al. [81] differentiated gasoline samples by applying multivariate pattern recognition

techniques to GC-MS data, including PCA and linear discriminant analysis.

Similarly, Tan et al. [82] successfully applied PCA and SIMCA to GC-MS data for IL classification, while Hupp et al. [83] looked at PCA of GC-MS data for discrimination of diesel fuels. Sigman et al. [84] differentiated gasoline samples in the same geographical region using covariance mapping and t-tests, and Doble et al. [85] applied PCA and artificial neural networks (ANN) for classification of premium or regular gasoline.

To date, no predictive weathering studies have been published for ILs, though this knowledge could prove valuable to forensic investigators. If we could pull patterns from weathered data that distinguish between fresh gasoline present before a fire and highly weathered gasoline, we could differentiate between an accidental spill occurring days prior to a fire and deliberate intent within hours of a fire. In reality, our focus is short-term predictions for IL spills due to the speed of evaporation. Ideally, narrowing down a time range for a fresh spill to within a few hours is our goal, as older spills would be indicative of an accident without the need for highly precise predictions.

1.3 Gas Chromatography

1.3.1 *One-dimensional gas chromatography*

Russian botanist Mikhail Tswett presented the concept of chromatography in 1903, publishing his research on the separation of plant pigments by liquid-adsorption chromatography in 1906 [86, 87]. The field was further developed in the 1940's by Martin and Synge [88], who won the 1952 Nobel Prize in chemistry for the invention of partition chromatography. Gas-liquid partition chromatography was introduced by Martin and James in 1952 when they used a gaseous mobile phase for the separation of volatile fatty acids [89]. Significant developments in GC continued with the introduction of capillary columns by Golay in 1957, followed by fused silica columns in 1979 by Dandeneau and Zerenner [90], which provided better efficiency and separation than packed columns. The developments continued, leading to heart-cut two-dimensional gas chromatography and finally to comprehensive two-dimensional gas chromatography [91]. Detailed histories of chromatography have been previously published by numerous authors including Ettre [92, 93] and Hinshaw [94].

Chromatography is a separation technique in which components are distributed between two phases, a stationary phase and a mobile phase. As the mobile phase passes over the stationary phase, analytes separate due to differential partitioning between these phases. As the interaction of analytes

with the stationary phase increases, their migration slows; likewise, if an analyte has greater affinity for the mobile phase, it will elute more quickly. In gas chromatography, the mobile phase is an inert gas and the stationary phase is typically a thin layer of liquid coated on the wall of a fused silica capillary or coated on inert solid support material packed into a column. Packed columns range from 0.5-10 m in length and have an internal diameter of 0.75-5.3 mm. Packed columns are not as widely used as wall-coated open tubular columns (WCOT), though applications include the separation of large sample sizes (packed columns contain more stationary phase) and the separation of gases such as oxygen and nitrogen. The research presented in this thesis was done on WCOT columns; there will be no further discussion of packed columns. WCOT columns have lengths varying from 1-30 m, are 0.1-0.53 mm in internal diameter and have a film thickness of 0.1-5.0 μm . These columns are connected on one end to a pressurized, heated injection port in which the sample is vaporized upon introduction. The carrier gas elutes the sample through the column, heated by the oven compartment, where it is then analyzed by a detector connected to the end of the column [95, 96, 97] (Figure 1-1).

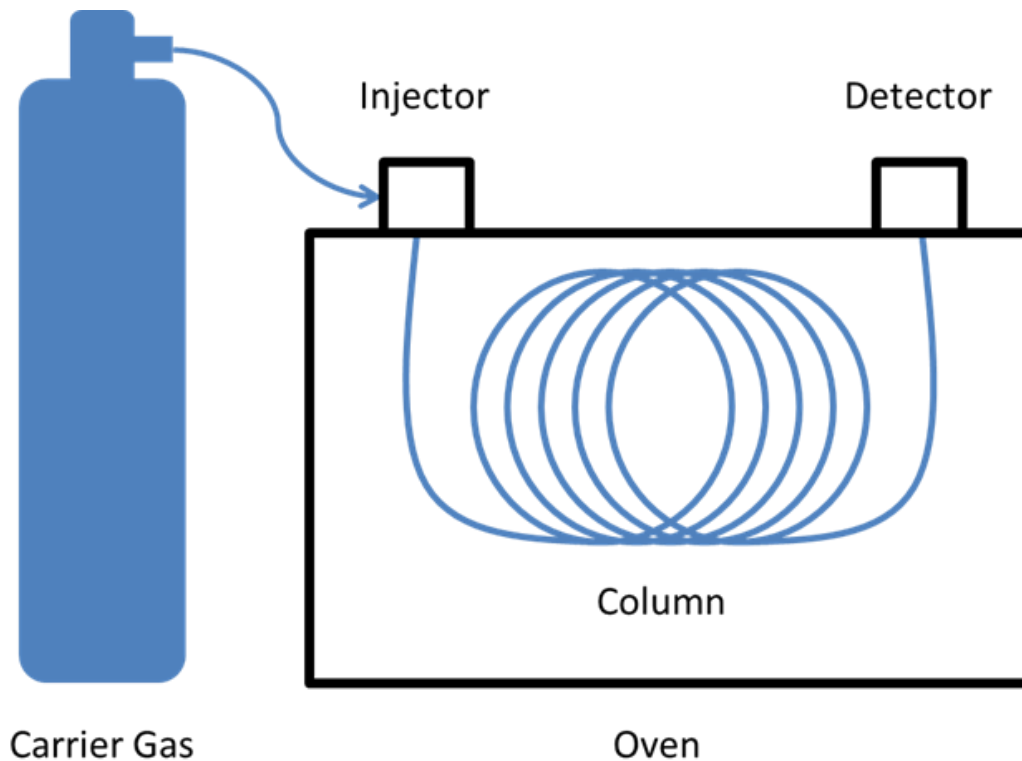


Figure 1-1. Schematic of a one-dimensional gas chromatograph.

The distribution coefficient (K_c) controls the rate of migration (Equation 1-1) in that analytes with large K_c are more retained by the stationary phase, and separation is achieved when analytes have different K_c values. The distribution coefficient is defined as the ratio of the equilibrium concentration of analyte in the stationary phase ($[A]_s$) to the equilibrium concentration of analyte in the mobile phase ($[A]_M$). In Equation 1-1, the retention factor (k) is calculated by dividing the mass of analyte in the stationary phase by the mass of analyte in the mobile phase. The phase ratio (β) represents the ratio of mobile phase volume (V_M) to stationary phase volume (V_S). Each of these values can be further broken down into simpler terms, as shown in Equations 1-2 and 1-3.

$$K_c = \frac{[A]_S}{[A]_M} = k\beta \quad (1-1)$$

$$\beta = \frac{V_M}{V_S} = \frac{r_c}{2d_f} \quad (1-2)$$

$$k = \frac{t_R - t_M}{t_M} \quad (1-3)$$

Retention time (t_R), is defined as the time required for an analyte to elute from a column and the dead time or hold-up time (t_M), is the time required for an unretained compound to elute from a column; both are required for calculating the retention factor [98] (Equation 1-3). The phase ratio can be calculated (Equation 1-2) using the column specifications provided by the manufacturer; the internal radius of the column (r_c) and the stationary phase film thickness (d_f). The distribution coefficient is temperature dependent. At higher temperatures, K_c becomes smaller and the analyte is less retained on the column (shorter t_R). For this reason, many chromatographers use temperature programming. As the temperature increases during a run, the K_c for less volatile compounds begins to decrease until these compounds elute from the column. Thus, temperature programming facilitates the timely separation of compounds within a sample having a wide range of retention factors.

Resolution in chromatography is a measure of separation between adjacent peaks, relative to their peak widths [99, 100]. There are numerous ways to improve the resolution for two analytes, as shown in Equation 1-4. Plate

number (N) is a measure of column efficiency or sharpness of the peak, and is calculated with Equation 1-5, where w_b is the peak width at the baseline. Efficiency can be increased by lengthening the column (which also increases analysis time), narrowing the column diameter, or increasing the film thickness of the stationary phase. Increasing the retention factor can also increase resolution. This is accomplished by lowering the temperature of the column, however it also increases analysis time and broadens peaks, affecting their detectability; it is also only effective to a certain point (approximately $k=10$), after which an increase in k has no noticeable influence. Finally, resolution can be altered with α , the selectivity factor, which involves altering analyte-stationary phase interactions by changing the chemistry of the stationary phase. The selectivity factor represents the difference in affinities for the stationary phase between a pair of analytes and is calculated as the ratio of retention factors for two adjacent peaks, with the later eluting peak as the numerator (Equation 1-6).

$$R_s = \left(\frac{\sqrt{N}}{4}\right) \left(\frac{k_2}{k_2+1}\right) \left(\frac{\alpha-1}{\alpha}\right) \quad (1-4)$$

$$N = 16 \left(\frac{t_R}{w_b}\right)^2 \quad (1-5)$$

$$\alpha = \frac{k_2}{k_1} \quad (1-6)$$

A final measure of system efficiency is peak capacity (n), the theoretical number of peaks that can be resolved by a given system in a given time [101, 102]. In one-dimensional chromatography, n is calculated by Equation 1-7 where t_{R_max} is the maximum retention time of your system. Unfortunately the peak capacity calculated for a system is not statistically possible to achieve due to the probability of peaks overlapping [103]. Increasing the separation power of a chromatographic system is possible however, when a two-dimensional system is implemented for sample analysis, as discussed in the next section.

$$n = \frac{t_{R_max} - t_M}{w_b R_S} \quad (1-7)$$

1.3.2 Two-dimensional gas chromatography

The concept of comprehensive two-dimensional gas chromatography (GC×GC) was first proposed by Giddings in 1984 [104, 105], but was first implemented in 1991 by Liu and Phillips [106]. The advantage of GC×GC over one-dimensional (1D) GC, is that the peak capacity is increased from that of a single column (n) to the product of the individual peak capacities of both dimensions ($n_1 \times n_2$). There is also an increase in sensitivity due to compression of the effluent band by the modulator separating the two columns [107, 108]. The modulator can also reduce chemical noise from the injector and primary column by focusing and then resolving it from the analyte peaks in the secondary column, with the final result being a simultaneous increase in signal and

decrease in noise. Finally, this technique provides ordered chromatograms which group structurally related compounds together, facilitating characterization of a sample (Figure 1-2).

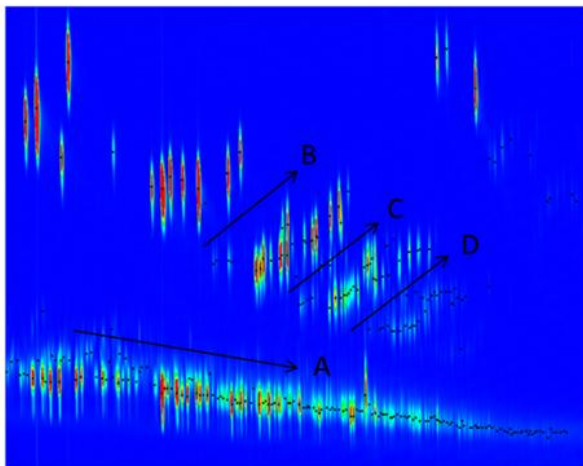


Figure 1-2. A chromatogram of gasoline demonstrating ordered elution. Arrow A represents alkanes and alkenes eluting with increasing molecular weight; arrows B, C and D represent aromatic compounds that elute with increasing molecular weight (left to right) and increasing polarity (bottom to top).

For the separation space to be maximized in a two-dimensional separation, it is important for the columns to be orthogonal, that is, we need the dimensions to operate with different retention mechanisms [109]. Furthermore, for a technique to be comprehensive, it requires that a representative fraction of the entire sample be separated by all dimensions and that each dimension preserve the separation achieved in any previous dimensions. Comprehensive techniques should not be confused with multidimensional techniques. For example, heart-cut GC is a multidimensional technique in which small, carefully

chosen fractions or cuts of the first-dimension effluent are redirected to a secondary column, resulting in a theoretical peak capacity that is the sum of the two individual columns (n_1+n_2). In this case, heartcut is considered multidimensional due to the use of multiple columns, but not comprehensive due to the fact that the secondary separation is only performed on a specific portion of the chromatogram.

As shown in Figure 1-3, GC×GC consists of two columns coupled together by a modulator or interface. The primary column is traditionally the same high resolution column used in 1D GC, usually 15-30 m long, 0.25-0.32 mm in diameter and 0.1-1 μm in film thickness. Typically the primary column employs a non-polar stationary phase resulting in an approximate boiling point separation for hydrocarbons; more specifically, separation is due to dispersion or London forces between the stationary phase and the analytes. The modulator collects fractions from the first column, focuses the fraction and releases it onto the second column in a short pulse. It is this refocusing in the second dimension that provides increased sensitivity for this technique and allows compounds co-eluting in the first dimension to be separated in the second. It has previously been determined that each peak eluting from the first dimension should be sampled a minimum of three to four times to preserve the primary separation [110].

The second-dimension separation is usually short and considered to be isothermal, with a polar stationary phase for specific interactions that are orthogonal to the primary column. Typical dimensions are 0.5-2 m long, 0.1 mm in diameter and 0.1 μm in film thickness. The need for a fast second-dimension separation is to prevent the wraparound of peaks. This phenomenon occurs when the retention time of a peak in the second dimension is longer than the modulation period, resulting in peak elution during a later modulation pulse than expected. This can cause a co-elution problem if the peak elutes in occupied space.

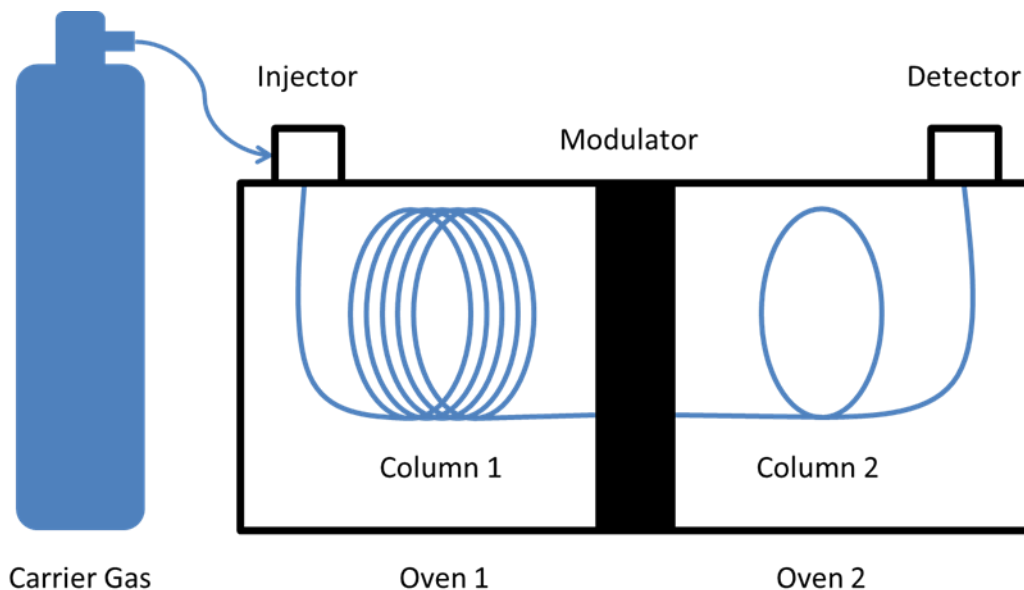


Figure 1-3. Schematic for a GCxGC

The key to comprehensive two-dimensional separations is the use of a thermal- or valve-based modulator. Thermal modulators come in a myriad of designs. The rotating thermal modulator was an early creation of Phillips and

co-workers [111, 112], though it was eventually replaced by cryogenic modulators due to the inherent problems associated with moving parts and the temperature limits instilled by requiring the modulator temperature to exceed the oven temperature by 100 °C. Marriott and Kinghorn developed the longitudinally modulated cryogenic system (LMCS) using liquid CO₂ to trap analytes [113]. This was followed by various designs using cold jets of liquid CO₂ or liquid nitrogen to trap analytes [114, 115, 116]. These cold jet modulators trap effluent from the first dimension by cooling the capillary with a cryogen, either causing K_c to increase and analyte to partition into the stationary phase, or by freezing the analyte in place. The trapped compounds are released when the cryogen is no longer pumped onto the capillary and the capillary is heated by the oven or a heating jet which pumps hot air onto the capillary (Figure 1-4).

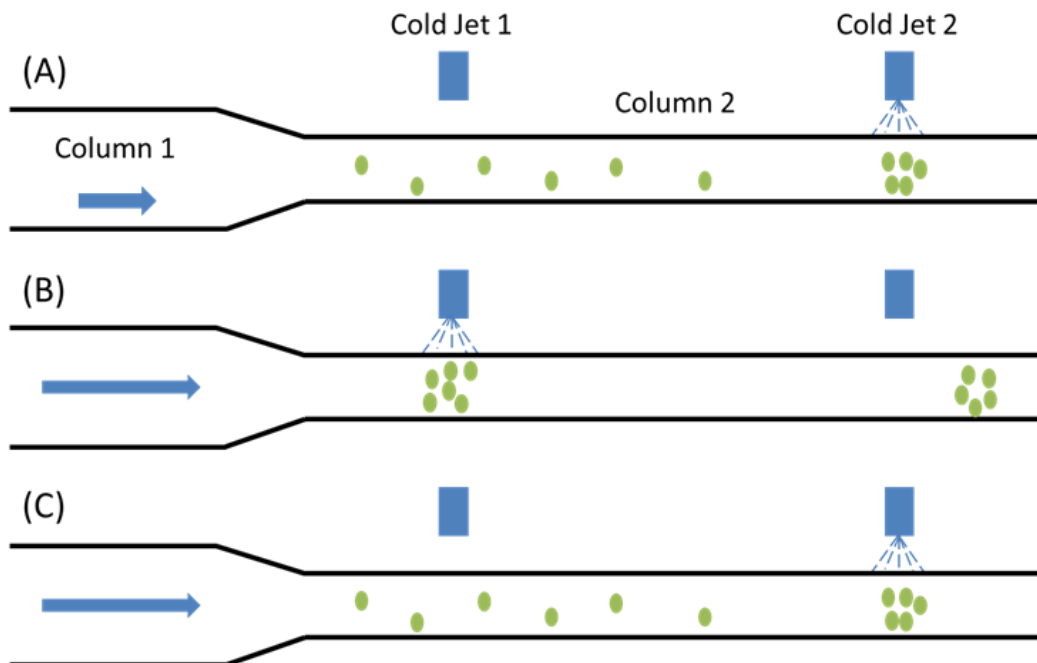


Figure 1-4. Cold Jet 2 cools the capillary and traps the analyte (A). Cold Jet 1 begins cooling the capillary and trapping analytes, preventing breakthrough while Cold Jet 2 is off and the trapped analytes begin moving down the column (B). The process repeats as Cold Jet 2 begins cooling and trapping analytes and Cold Jet 1 is off to allow analytes to reach Cold Jet 2 (C).

The original valve-based interfaces were designed so the primary column effluent alternates between the secondary column and venting to the atmosphere. This approach is less sensitive than thermal modulation due to the lack of band compression that occurs during thermal focusing, as well as partial loss of analytes during venting. Valves have the advantage of not using expensive cryogens, but do have low temperature limits which can hinder separation of high molecular weight compounds. More recently, Bueno and Seeley developed a dual-sample-loop system in which the entire sample is transferred to the second column and the valve is not in the sample flow path, but outside the

oven, allowing for increased temperatures [117]. In this case, however, the sample loop volumes must be balanced with flow rates and modulation period to avoid over-filling of loops. Changes in operating conditions with this modulator usually necessitate a change in sample loop volume.

Once eluent bands are refocused in the modulator, the resulting peak widths are 100-600 ms in the second dimension. Generally we want a minimum of ten points across the peak width for accurate peak integration. These narrow peaks require a detector with a small internal volume and an acquisition rate of 50-200 Hz. Detectors with these specifications are generally limited to the FID, micro-electron capture detectors (μ ECD) and TOFMS. The FID has a negligible internal volume and acquisition rates up to 300 Hz; this detector responds to most hydrocarbons but is insensitive to non-hydrocarbons such as noble gases, N_2 , O_2 , CO , CO_2 , and NO . The μ ECD has a 150 μ L internal volume and adequate acquisition rates; this detector is sensitive to halogen- and nitrogen-containing molecules but fairly insensitive to hydrocarbons. A TOFMS provides the necessary acquisition rates by simultaneously sampling all mass-to-charge ratios and provides structural information for identification. Though many other selective detectors have been reported in the literature [118, 119, 120], these are the most commonly used for GC \times GC.

Data analysis for GC \times GC involves translating the linear one-dimensional data collected by the detector, into the three-dimensional plots characteristic of

this technique. The linear data observed by the detector are a continuous series of second-dimension separations. Data processing software slices the data into individual second-dimension chromatograms which are then aligned side-by-side with the primary retention time set as the x-axis, secondary retention time as the y-axis and detector signal as the z-axis. The data are most frequently viewed as a contour plot for easy interpretation (Figure 1-5). Integration is achieved by summing the individually modulated peaks which comprise a single peak (3-4 modulations per individual peak). A more detailed review on data interpretation was published by Harynuk et al. [121].

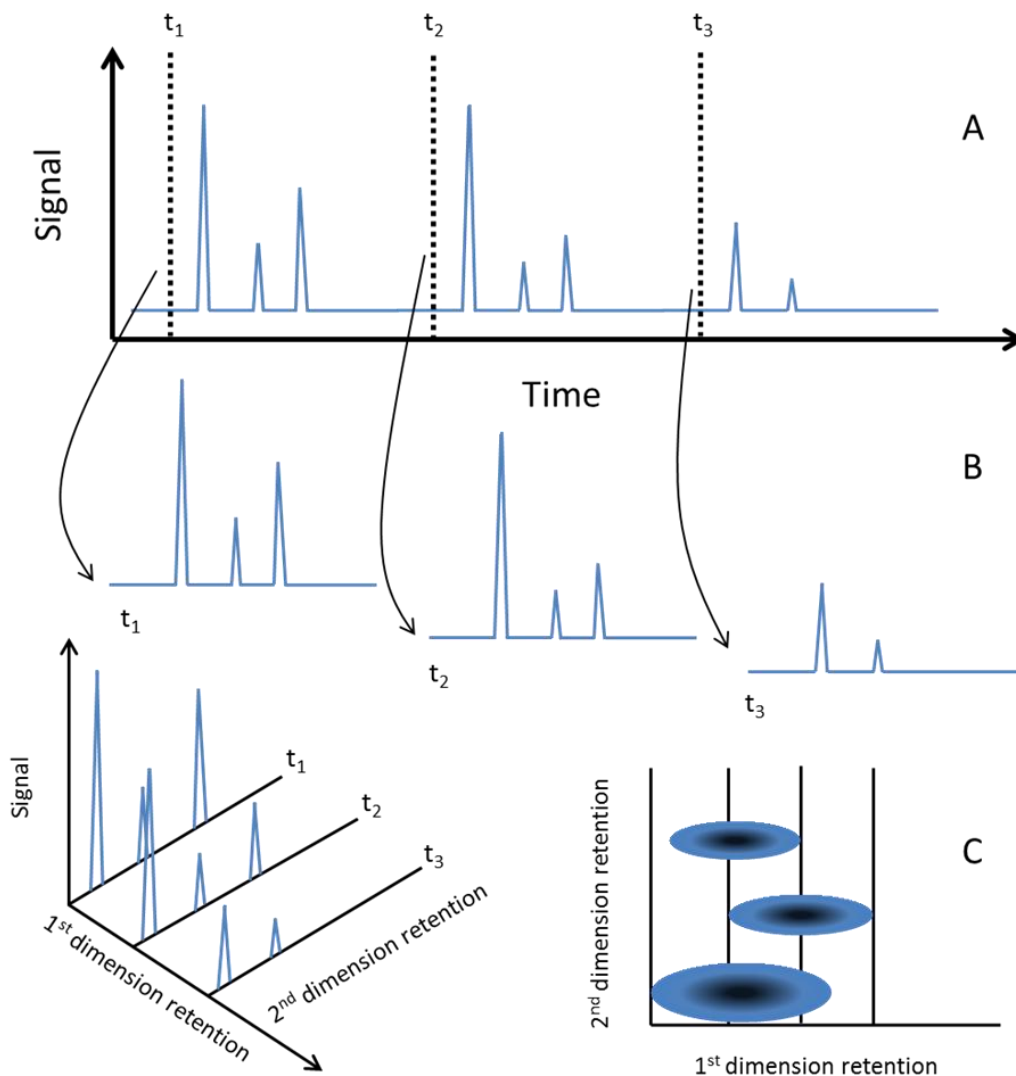


Figure 1-5. Analysis of two-dimensional chromatographic data. The detector records a series of sequential second-dimension chromatograms (A); the linear signal is sliced into individual second-dimension chromatograms (B); individual chromatograms are aligned with the first-dimension retention time as the x-axis and the second-dimension retention time as the y-axis and signal intensity as the z-axis. The standard convention is to then view the data as a contour plot viewed top-down (C). Adapted from Figure-4 in reference [102].

The field of multidimensional chromatography continues to expand in function and application. For example, interest in building upon the principles of comprehensive GC×GC has been shown by Watson et al. [122], as well as Ledford

and Billesbach's research into three-dimensional GC [123]. However, to further establish the basic concepts of GC×GC instrumentation, detailed reviews have been published by Górecki et al. [124], Ong and Marriott [125], Dallüge et al. [126] and Adahchour et al. [127]; as well, reviews on recent developments in GC×GC have been published by Adahchour et al. [128, 129]. Moreover, numerous reviews on the widespread applications of GC×GC have been covered by Marriott and Shellie [130], and Adahchour et al. [131, 132].

What these reviews will serve to highlight is the history of GC×GC in the analysis of petroleum, and its advantages of ordered chromatograms and peak capacities; these qualities make GC×GC a logical choice for the analysis of weathered gasoline, as covered in Chapter 3. However, before delving into the complex analysis of weathered petroleum, Chapter 2 will discuss the use of one-dimensional GC in a proof-of-concept study of a weathered model mixture of volatile hydrocarbons.

1.4 References

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2. Estimation of the age of a weathered model mixture of volatile organic hydrocarbons¹

2.1 Overview

Hydrocarbon pollution from accidental release or natural seepage can cause damage with far reaching environmental and financial repercussions. Consequently, liability associated with petroleum release in the environment requires reliable characterization and source identification. This is complicated by weathering, which encompasses the physical, chemical and biological processes responsible for hydrocarbon degradation. Extensive research has been conducted to improve our understanding of the compositional changes that occur during heavy petroleum weathering, which is essential to determining the fate and behaviour of oil spills in the environment [1, 2, 3, 4]. Unfortunately, few studies have focused on petroleum weathering with the aim to estimate the time of exposure based on the observed composition of a weathered sample at a given time, and assuming a prior composition. This chapter describes a proof-of-concept study which assessed the feasibility of estimating the age of petroleum mixtures by applying multivariate techniques to the one-dimensional gas chromatographic profiles of a weathered model hydrocarbon mixture. Once our chemometric models were validated, this research was expanded to a more complex petroleum mixture, discussed in Chapter 3.

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2.2 Experimental

2.2.1 *Weathering chamber*

An enclosed chamber was built to control and adjust the major weathering parameters of temperature and airflow (Figure 2-1). The chamber, built of stainless steel, measured 51×25×34 cm (length×width×height). Access to the chamber was provided by a sliding front panel. The chamber contained three perforated-metal shelves, two of which were removable, and six through-ports in the chamber roof for thermocouple access. The chamber was insulated on all sides by a 2.5 cm thick Styrofoam™ layer and it sat on a 3 mm thick rubber mat. The chamber temperature was regulated by a recirculating water bath that pumped heated water through a serpentine grid of 1/4 inch copper tubing that rested on the chamber floor. After passing through the chamber, the water entered the core of a 2 L cylindrical water jacket before returning to the water bath. High-pressure laboratory air was passed through a hydrocarbon trap and then counter-currently (to the water flow) through a coil of 1/4 inch copper tubing that was soldered around the outside of the water jacket, bringing the air to a set temperature. The tubing then passed into the bottom of the chamber and followed a serpentine path with a series of ~0.5 mm diameter holes in the tubing to distribute the air evenly throughout the chamber. Air that entered the chamber was vented through a segment of 2-inch pipe connected to the top of

the chamber and into a fume hood. The water jacket and all copper tubing were insulated with foam insulation.

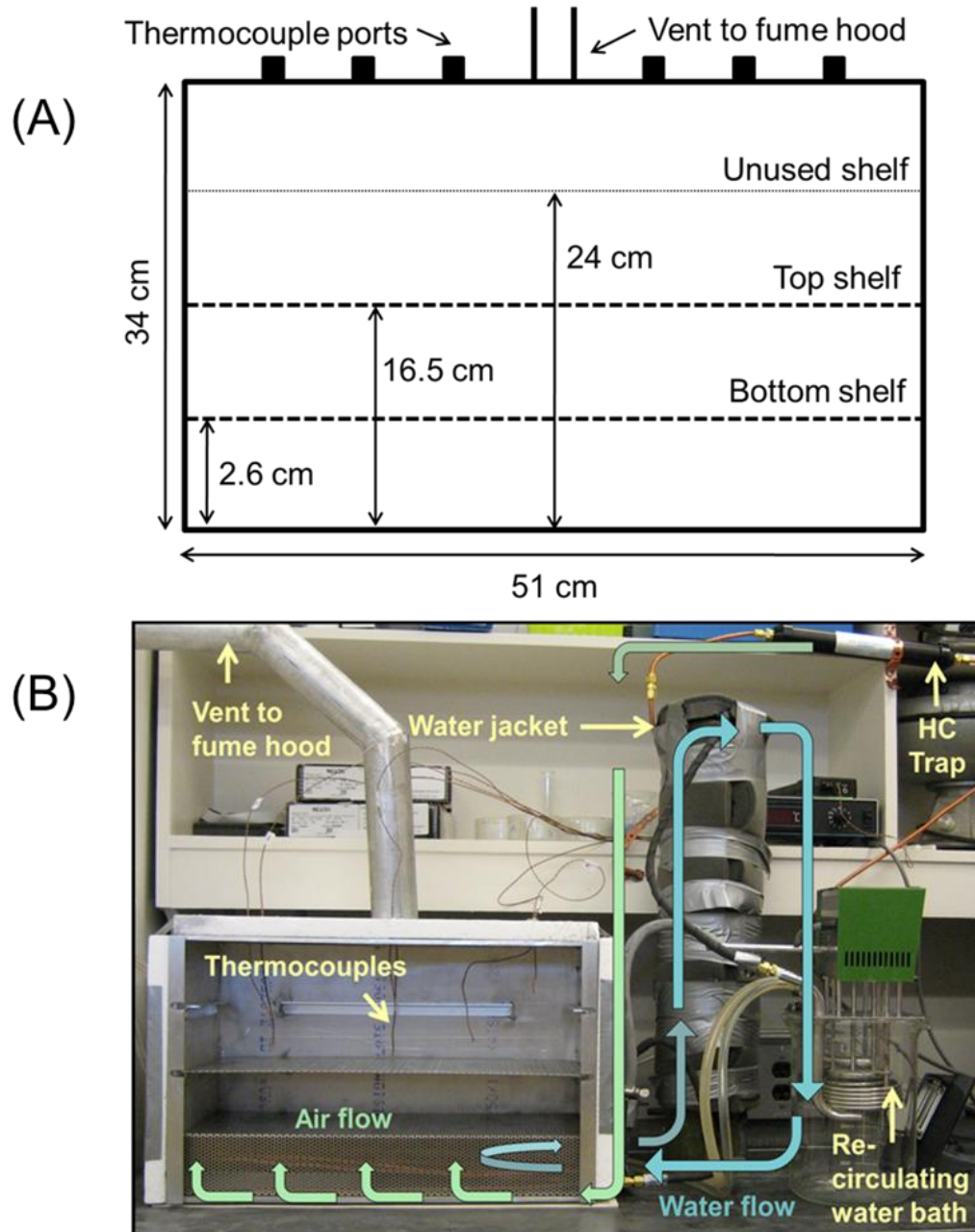


Figure 2-1. Schematic of the weathering chamber constructed to control temperature and airflow during weathering studies (A); photograph of the chamber (B).

2.2.2 *Materials and reagents*

Nine compounds were chosen for the model hydrocarbon mixture, each one representing a characteristic component of gasoline [5, 6]. The nine-compound model hydrocarbon mixture was made by combining 10 g of naphthalene (Caledon, ON, Canada) and 30 mL each of the following: benzene (Caledon), heptane (Caledon), 2,2,4-trimethylpentane (Chemical Samples Co., OH, United States), toluene (Fisher Scientific, ON, Canada), m-xylene (Sigma-Aldrich, ON, Canada), nonane (Sigma-Aldrich), decane (Sigma-Aldrich) and 1,2,3,5-tetramethylbenzene (Sigma-Aldrich).

For weathering, 50 mL aliquots of the sample solution were poured into circular Pyrex[®] dishes (80×40 mm) and placed on a shelf in the weathering chamber. Samples of the weathered solution were collected at varying times during the course of the five-day weathering study. Samples were collected every half-hour within the first two hours of weathering, followed by hourly increments until six hours total time had elapsed, and then two-hour increments until 12 hours had elapsed. At this time, eight-hour increments were implemented until 36 hours had elapsed, then twelve-hour intervals until 84 hours had elapsed. A final sample was taken at 108 hours total elapsed time. A total of twenty samples were collected from each dish and stored at -4 °C in sealed 1.8 mL GC sample vials. Prior to analysis, weathered samples were brought to room temperature and diluted 200× using pentane (Fisher Scientific)

containing 3,6-dimethyloctane (Chemical Samples Co.) as an internal standard (IS) at a concentration of $0.5 \mu\text{L}\cdot\text{mL}^{-1}$.

2.2.3 GC-MS analysis

Samples were analyzed using an Agilent 7890 gas chromatograph coupled to an Agilent 5975 mass spectrometer (Agilent Technologies, ON, Canada). A $30 \text{ m}\times 0.25 \text{ mm}\times 0.25 \mu\text{m}$ HP-5 column (Agilent Technologies) with helium carrier gas at a constant pressure of 9.5 psi was used. The total run time was 10.7 minutes with an oven program of $35 \text{ }^\circ\text{C}$ (hold 3 min) to $120 \text{ }^\circ\text{C}$ at $15 \text{ }^\circ\text{C}\cdot\text{min}^{-1}$, then to $180 \text{ }^\circ\text{C}$ at $30 \text{ }^\circ\text{C}\cdot\text{min}^{-1}$. The front inlet temperature was held at $250 \text{ }^\circ\text{C}$ and the transfer line temperature was held at $185 \text{ }^\circ\text{C}$. The sample injection volume was $1 \mu\text{L}$, using a 500:1 split ratio. Electron impact ionization (70 eV) was used with a quadrupole mass analyzer in full scan mode (35 to 250 amu).

2.2.4 Data analysis

All compound peak areas were integrated using ChemStation™ software (Agilent Technologies). Data were then analyzed using MATLAB 7.9 (The MathWorks™, MA, United States) and PLS Toolbox 5.8.2 (Eigenvector Research Inc. WA, United States).

2.3 Results and discussion

Two weathering studies were conducted in which two dishes each were placed on the top (Dishes A and B) and bottom (Dishes C and D) shelves of the weathering chamber. A sample was collected from each dish at the designated time using a Pasteur pipette. The chamber temperature was monitored with five evenly spaced thermocouples. For the first study in September 2009, the chamber was held at 25 ± 1 °C with a constant flow rate of $11.8 \text{ L}\cdot\text{min}^{-1}$ (16 chamber volumes per hour). The second study, held in October 2009, was conducted under conditions that were identical to the prior study, with the one change being a more precise thermocouple meter which provided measurements to 0.1 °C. During this study, the chamber was held at a constant temperature of 26.7 ± 0.5 °C.

During these studies we noticed that the dishes on the bottom shelf (C and D) experienced a faster weathering rate than the top shelf (A and B). This can be explained by two observations. Firstly, the clean air entered from the bottom of the chamber and passed around the dishes on the bottom shelf first. Consequently, when the air reached the top shelf, it may already have contained a significant amount of evaporated sample mixture, slowing the evaporation from the upper dishes. Secondly, the temperature was observed to be slightly higher on the bottom shelf than the top shelf (0.7 ± 0.5 °C), which would slightly increase evaporation rates for compounds in the bottom dishes. Samples from

either shelf can be modeled successfully, but for simplification during model construction, we arbitrarily chose the data collected from the top shelf for our model studies.

All samples were analyzed in triplicate on a gas chromatograph coupled to a mass spectrometer (GC-MS), resulting in a total of sixty data points from each dish. Before evaluating any chemometric models, the integrated area of each peak was normalized to the area of the internal standard (to account for variations in GC injection volume) then divided by the normalized total peak area. We evaluated numerous preprocessing techniques during model calculation, including autoscaling and mean centering, but found the data responded well to a combination of autoscaling and generalized least squares weighting (GLSW) [7].

Mean-centering is a common preprocessing technique in which the mean of each column is subtracted from all the values found in that column. Autoscaling is another common preprocessing technique which mean-centers the data, followed by dividing each column by its standard deviation. This gives each column a mean of zero and a standard deviation of one, resulting in all variables having equal influence on the calculation of a model. GLSW is a much less commonly used technique that down-weights the differences between replicate measurements. Once a preprocessing technique was chosen, various chemometric methods were explored including partial least squares (PLS),

non-linear PLS (PolyPLS) and locally weighted regression (LWR). Table 2-1, located in Section 2.3.3, compares the three preprocessing techniques and their effects on model prediction.

2.3.1 *GLSW algorithm*

GLSW uses the eigenvectors and eigenvalues of a covariance matrix to down-weight signal identified as being from known interferences or differences between samples which should otherwise be the same, giving this technique a wide variety of applications. Martens et al. [8] have used this technique to preprocess spectrophotometric data, making the instrument blind to unwanted interferants while retaining analyte sensitivity. Blake et al. [9] used a target detection algorithm based on generalized least squares to distinguish between nitro-containing compounds stained on steel plates. This was done by comparing the images recorded using a commercial long-wave infrared imaging spectrometer and comparing those images to the target spectra of the compounds using laboratory reflection spectra. Similarly, Burr et al. [10] also used hyperspectral long-wave infrared imagery for detection and identification of chemical plumes by comparing to a library of known chemicals. Gallagher et al. [11] have also used generalized least squares for target detection of chemical spills using mid-infrared reflection spectroscopy.

In this work, X-block variance is identified for down-weighting using a sorted list of the reference values (Y-block). To a first approximation, the

reference values can be considered a description of the similarity between samples. Samples with similar y -values would be expected to have similar responses (rows of the X-block). In order to identify the differences between samples with similar y -values, the rows of both the X- and Y-blocks are simultaneously sorted in order of increasing y -value. This puts samples with similar y -values near each other in both blocks. Next, the difference between proximate samples is determined by calculating the derivative down each column of the X-block. These derivatives are calculated using a 5-point, first-order, Savitzky-Golay first derivative. This derivative yields a matrix, \mathbf{X}_d , in which each sample (row) is an average of the difference between it and the four samples most similar to it. A similar derivative is calculated for the sorted Y-block, yielding vector \mathbf{y}_d , a measure of how different the y values are for each group of five samples.

At this point, \mathbf{X}_d could be used to calculate the covariance matrix for down-weighting. However, some of the calculated differences (rows) may have been performed on groups of samples with significantly different y values. These rows contain features which are more correlated to the Y-block and should not be removed by GLSW. To avoid this, the individual rows of \mathbf{X}_d need to be re-weighted by converting the sorted Y-block differences into a diagonal re-weighting matrix, \mathbf{W} , in which the i^{th} diagonal element, w_i , is calculated from the rearranged equation:

$$\log_2(w_i) = -y_{d,i} s_{yd} \quad (2-1)$$

The value $y_{d,i}$ is the i^{th} element of the \mathbf{y}_d vector, and s_{yd} is the standard deviation of y-value differences:

$$s_{yd} = \sqrt{\frac{\sum_{i=1}^m (y_{d,i} - \bar{y}_d)^2}{m-1}} \quad (2-2)$$

The re-weighting matrix is then used along with \mathbf{X}_d to form the covariance matrix

$$\mathbf{C} = \mathbf{X}_d^T \mathbf{W}^2 \mathbf{X}_d \quad (2-3)$$

and followed by the singular-value decomposition of the matrix, which produces the left eigenvectors, \mathbf{V} , and the diagonal matrix of singular values, \mathbf{S} :

$$\mathbf{C} = \mathbf{V} \mathbf{S}^2 \mathbf{V}^T \quad (2-4)$$

Next, a weighted, ridged version of the singular values is calculated

$$\mathbf{D} = \sqrt{\frac{\mathbf{S}^2}{\alpha} + \mathbf{I}_D} \quad (2-5)$$

where \mathbf{I}_D is a diagonal matrix of ones of appropriate size and α is the weighting parameter. A value of α is chosen, usually between 1 and 0.0001, to define the level of influence the filter has on the X-block. At large values ($\alpha > 1$), the filter has less effect and its influence increases as α decreases. Finally, the

inverse of these weighted eigenvalues are used to calculate the filtering matrix, G :

$$G = VD^{-1}V^T \quad (2-6)$$

This filtering matrix can be used by simply projecting a sample into the matrix. The result of this projection is that correlations present in the original covariance matrix are down-weighted (as defined by α) while other variances pass. The filtering matrix is used both on the original training data prior to model calculation, and any new data predicted with the regression model.

2.3.2 Classification of weathered samples using PLS-DA

Though only nine variables are used, the weathering profiles of individual compounds are collectively complex (Figure 2-2) (raw data are tabulated in Appendix A). Multiple linear regression (MLR) and PLS were initially explored for modeling across the entire time range, but the results were unsatisfactory. For example, MLR made predictions with an error of 185 minutes and PLS had a prediction error of 244 minutes for all samples, including the most lightly weathered. This is likely due to the fact that the weathering patterns for the different compounds do not vary linearly with time (or the natural logarithm of time). To simplify matters, the data were split into two classes for lightly weathered and highly weathered samples. Within each of these two groups the data were found to be somewhat linear, so partial least squares discriminant

analysis (PLS-DA) was used as a classification tool to determine to which group the samples belonged. PLS-DA seeks to find factors or latent variables (LVs) in multivariate space that discriminate between classes in the calibration set by using a PLS model and calculating a Bayesian threshold, where the number of false positives/negatives is minimized for the prediction of new data.

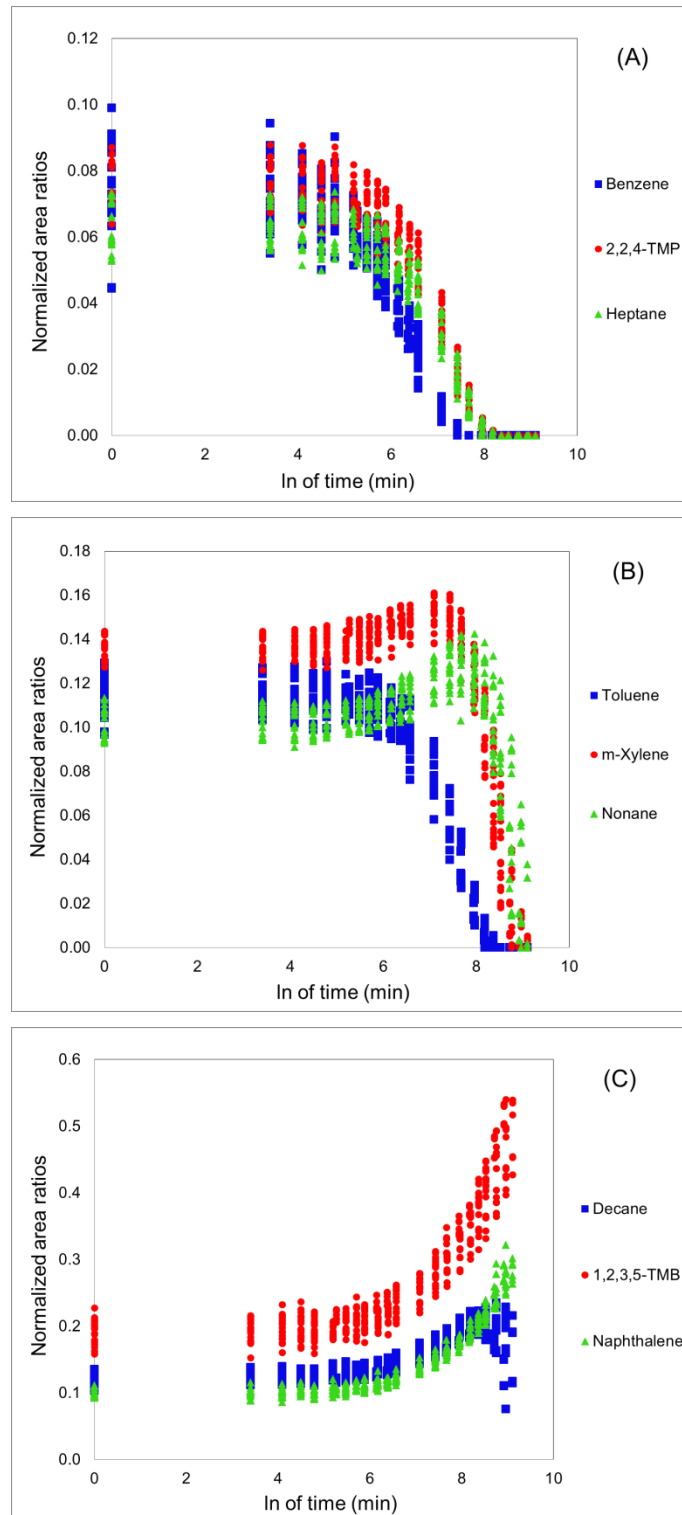


Figure 2-2. Weathered profiles for the model mixture (combined studies). The x-axis represents the natural log of time (min) samples were collected and the y-axis is the normalized peak areas divided by the normalized total peak area. (A) shows benzene, 2,2,4-trimethylpentane and heptane weathering; (B) shows toluene, m-xylene and heptane; (C) shows decane, 1,2,3,5-tetramethylbenzene and naphthalene weathering.

The weathered samples were divided into two classes. Class 1 was designated for samples weathered 0-12 hours (Samples A and B, 1 through 12), and Class 2 was 20-100 hours (Samples A and B, 13 through 20). Each replicate measurement taken was treated individually, resulting in a 120 (sample) by 9 (variable) X-block matrix for each of the individual weathering studies and a 240 by 9 X-block for the combined studies. Six different training/test sets were created from the original data matrices by randomly removing samples to use for model validation (test set). Of the 120 samples from each weathering study, 80 were randomly chosen to form the training set and 40 were chosen as a test set. Similarly, of the 240 samples from the combined weathering studies, two-thirds formed the training set and one-third formed the test set. The training sets were preprocessed by autoscaling and cross-validated using random subsets during model calculation. All training sets for the September data were optimized with three LVs, October training sets optimized with two LVs, and the combined training sets optimized with two LVs. All models successfully separated the classes and correctly classified the test samples in all six training/test sets (Figure 2-3, Figure 2-4 and Figure 2-5). These results indicate that PLS-DA is capable of separating classes whose individual samples originated from weathering studies held weeks apart and at slightly different temperatures.

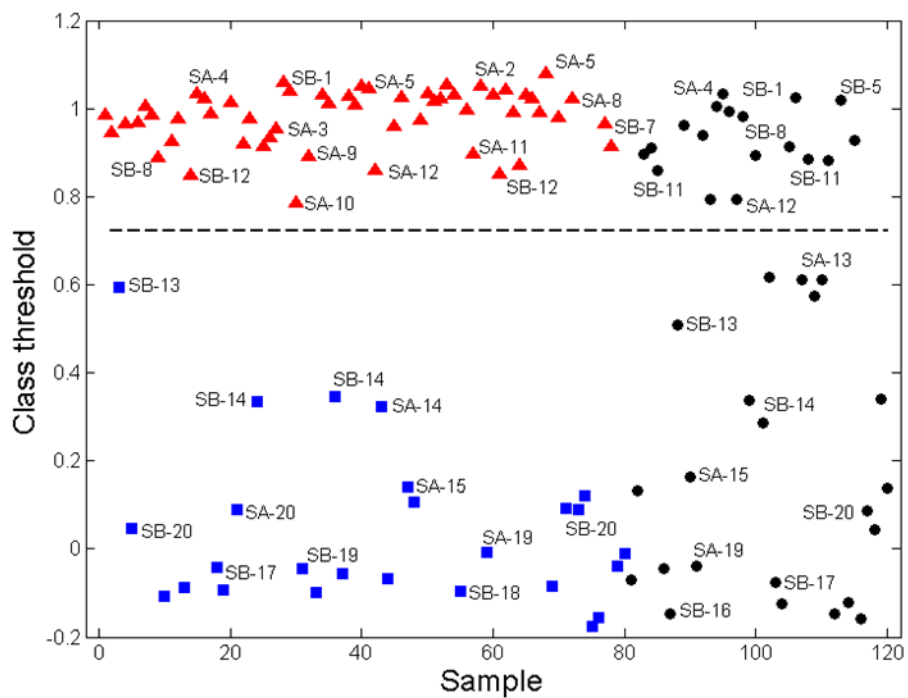


Figure 2-3. PLS-DA of a September training/test set shows both classes are clearly separated by the class threshold and all test samples correctly classified; Class 1 training set represented by red triangles; Class 2 training set represented by blue squares; Validation test set represented by black circles. The samples are identified by weathering study, dish and sampling time (ex: SB-13 is the thirteenth sample taken from dish B for the September study).

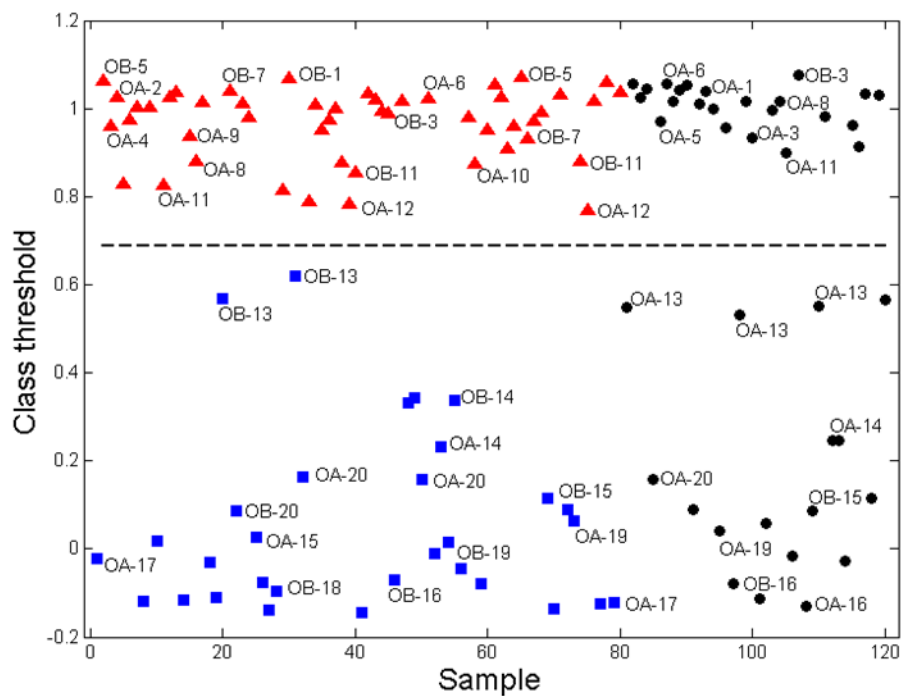


Figure 2-4. PLS-DA of an October training/test set shows both classes are clearly separated by the class threshold and all test samples are correctly classified; Class 1 training set represented by red triangles; Class 2 training set represented by blue squares; Validation test set represented by black circles. The samples are identified by weathering study, dish and sampling time (ex: OA-20 is the last sample collected from dish A for the October study).

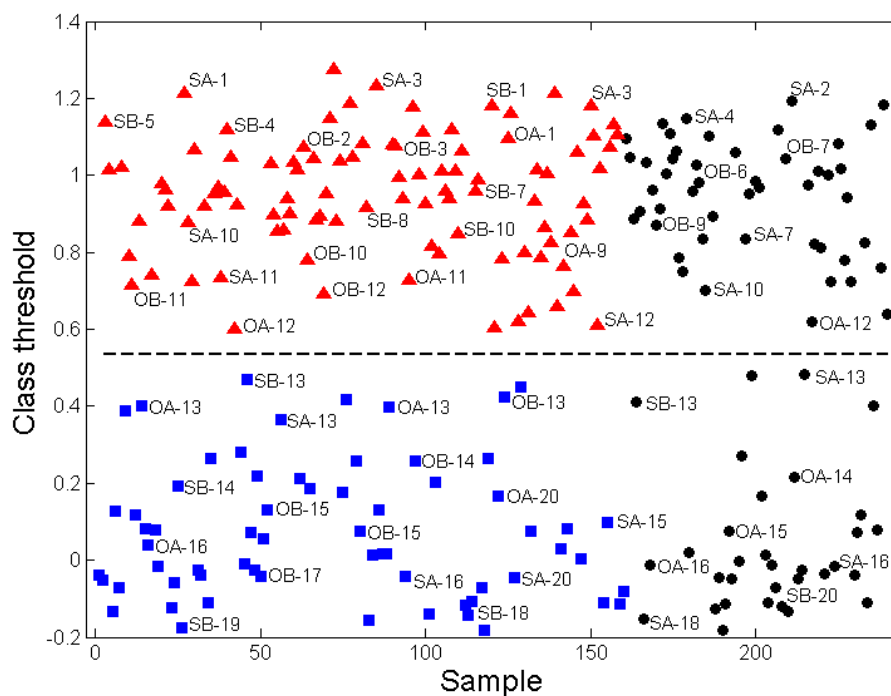


Figure 2-5. PLS-DA of a combined September and October training/test set shows clear separation between the classes and correct classification of the test samples; Class 1 training set represented by red triangles; Class 2 training set represented by blue squares; Validation test set represented by black circles.

2.3.3 PLS, PolyPLS and LWR

PLS seeks to find the LV, which captures the greatest variance in the independent variables (X-block) that is also relevant to predicting the dependent variables (Y-block), while assuming a linear inner relation between the X and Y-blocks. This is accomplished by decomposing the X-block into scores and loadings pairs, where loadings relate to the variables and scores relate to the samples; each pair being represented by a LV. Cross-validation of the training data using random subsets was used to estimate the optimum number of LVs for the model by reserving a fraction of the training set for internal validation.

From the original 120 by 9 X-block used for PLS-DA on the October and September studies, Class 1 samples (<12 hours exposure) reduced to a 72-sample matrix and the 240 by 9 matrix for the combined studies reduced to a 144-sample matrix. Class 2 (20-100 hours exposure) data sets reduced to a 48-sample matrix for the individual studies and a 96-sample matrix for the combined study. From each matrix, two-thirds of the samples were randomly chosen to form a training set for model calculation and the remaining samples formed a test set for model validation. This process was repeated to produce six different training/test sets for each matrix on which to build/validate a model. The corresponding time data were assigned to the Y-block. The X- and Y-matrices were preprocessed by autoscaling and performing GLSW with $\alpha = 0.01$.

The root mean square error of prediction (RMSEP) was used to gauge how well the models could predict new data [12]. Given by Equation 2-7, y_i is the true y-value for sample i , \hat{y}_i is the y-value predicted for sample i with the model under evaluation, and n is the number of samples for which a prediction is obtained.

$$RMSEP = \sqrt{\frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n}} \quad (2-7)$$

For the September, October, and combined Class 1 data, cross-validation resulted in an optimized PLS model with two LVs, across all training/test sets. Both the September and the combined models captured over

85% and 97% variance in the X- and Y-blocks respectively, while the October model captured over 93% and 98% variance. PLS was also applied to the Class 2 data, resulting in models optimized with three LVs for the September, October and combined data (across all training sets) that captured over 92% and 96% variance in the X- and Y-blocks of the individual studies, and over 89% and 97% variance in the combined studies.

PolyPLS is similar to PLS; however, the algorithm builds nonlinear models by using polynomial inner relations rather than assuming linearity as with PLS. The number of LVs found for the optimized PLS models were also used in building the nonlinear models, and both second- and third-order polynomial models were calculated. A second nonlinear regression technique explored was LWR. LWR is a smoothing procedure that uses local fitting to estimate a regression surface (Figure 2-6); it is particularly useful when the dependent variables have a nonlinear relationship with the independent variables [13, 14]. A subset of the calibration data is chosen to create the local regression window for an observed sample. The samples in each window are chosen based on their proximity to the observed sample, with closer samples having more influence on the placement of the local regression line. This process is repeated for each sample. Models are calculated using a defined number of LVs, a smoothing parameter, and a y-distance parameter. The smoothing parameter determines the fraction of total samples used in the local regression window. The y-distance parameter determines the method with which local points are chosen for the

regression window. A γ -distance of zero only considers samples that lie close in LV space, while values approaching one will also account for samples with similar Y-block values. A value of 0.8 was chosen for the γ -distance parameter in all models, while the smoothing parameter varied between 0.3-0.7 for each training set; both parameters were chosen through trial-and-error for all model calculations. For both classes, the number of LVs alternated between two and three, depending on the training set.

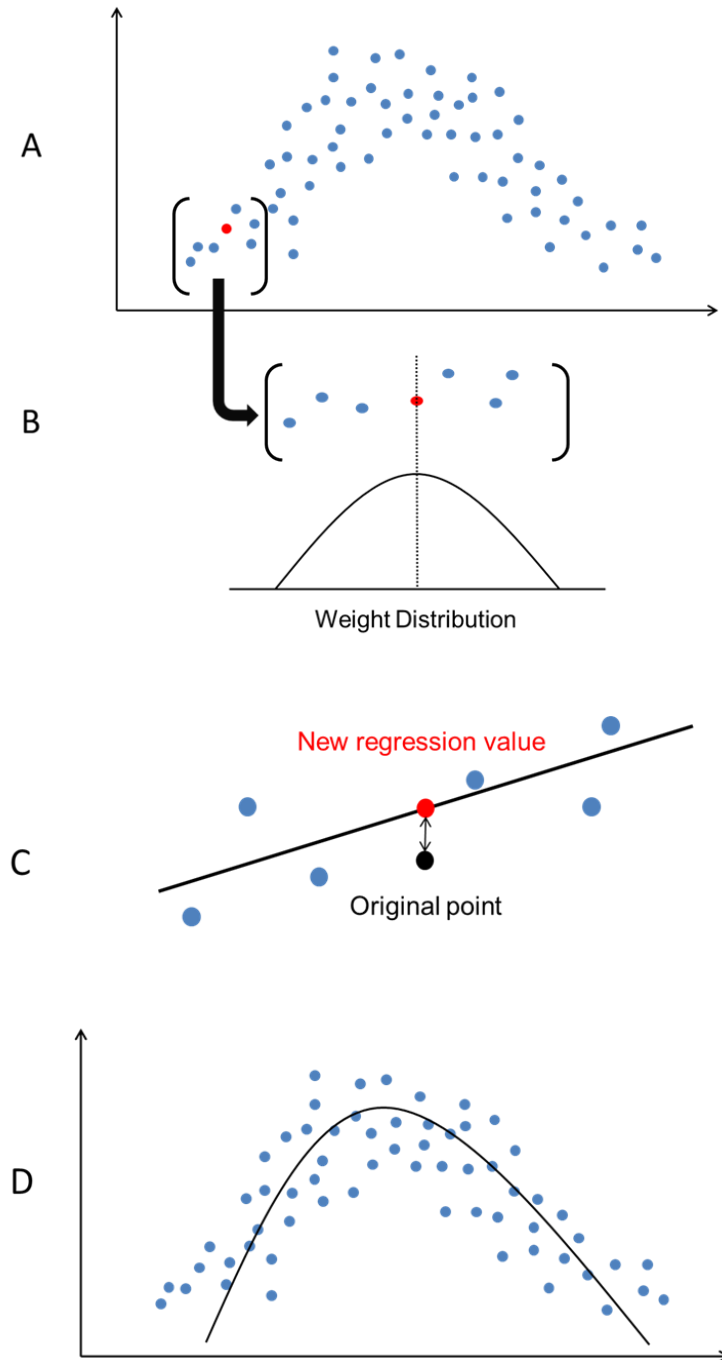


Figure 2-6. LWR performs regression around a point of interest, using the neighboring points found within the regression window (A). The points within the local regression window are weighted by proximity to the point of interest, with those closest to the point of interest (red point) having the most influence on the regression line (B). A weighted PLS model is fitted to the points in the regression window, using a defined number of LVs. A new regression value is then obtained for the point of interest (C). A regression value is obtained for all data points and a regression surface is estimated based on these regression values (D).

The results for all training/test sets were combined to provide a RMSEP range for each regression method as shown in Table 2-2. In general, we see that increasing the number of samples used to calculate a model by combining the September and October studies has a stabilizing effect, as seen by a narrowing of the RMSEP range. Moreover, we see a positive effect on the Class 2 models with the reduction in overall prediction error. A second-order polynomial model appears to more accurately predict Class 1 data than linear PLS; however, the model is less stable in its Class 2 predictions, as seen by the larger window of error. Similarly, we find that model performance is further hindered when a third-order polynomial is used, most likely due to overfitting of the calibration data.

Finally, LWR (Figure 2-7 and Figure 2-8) outperforms both PLS and PolyPLS regression methods, which becomes more apparent with the noticeably smaller and narrower RMSEP for Class 2. LWR is most likely best suited for our data because it is a nonparametric technique, meaning the model does not require a priori specification on the relationship between the X- and Y-blocks. As a result, the fit of the regression curve is obtained empirically, rather than through assumptions on the nature of the data which would produce a curve by calculating the coefficients of a pre-determined equation.

Table 2-1. The RMSEP for all regression models and preprocessing techniques explored.

	Class 1 (min)				Class 2 (h)			
	PLS	PolyPLS (2 nd)	PolyPLS (3 rd)	LWR	PLS	PolyPLS (2 nd)	PolyPLS (3 rd)	LWR
Autoscaling	49-58	43-50	46-52	36-44	4.8-5.6	4.2-6.2	4.4-5.8	3.1-4.2
Mean-centering	50-61	43-45	49-50	36-40	4.9-5.5	5.0-6.2	5.2-5.5	4.0-4.9
GLSW	38-48	36-43	35-48	28-39	3.9-4.6	3.8-5.0	4.0-5.7	3.6-4.2

Table 2-2. The RMSEP for all regression methods using GLSW as the preprocessing technique.

	Class 1 (min)				Class 2 (h)			
	PLS	PolyPLS (2 nd)	PolyPLS (3 rd)	LWR	PLS	PolyPLS (2 nd)	PolyPLS (3 rd)	LWR
September	27-44	27-38	31-39	26-40	3.7-4.7	2.9-5.4	4.1-7.5	1.8-3.7
October	24-35	23-33	25-37	22-32	4.3-6.7	4.4-7.1	4.7-8.5	3.3-5.6
Combined	38-48	36-43	35-48	28-39	3.9-4.6	3.8-5.0	4.0-5.7	3.6-4.2

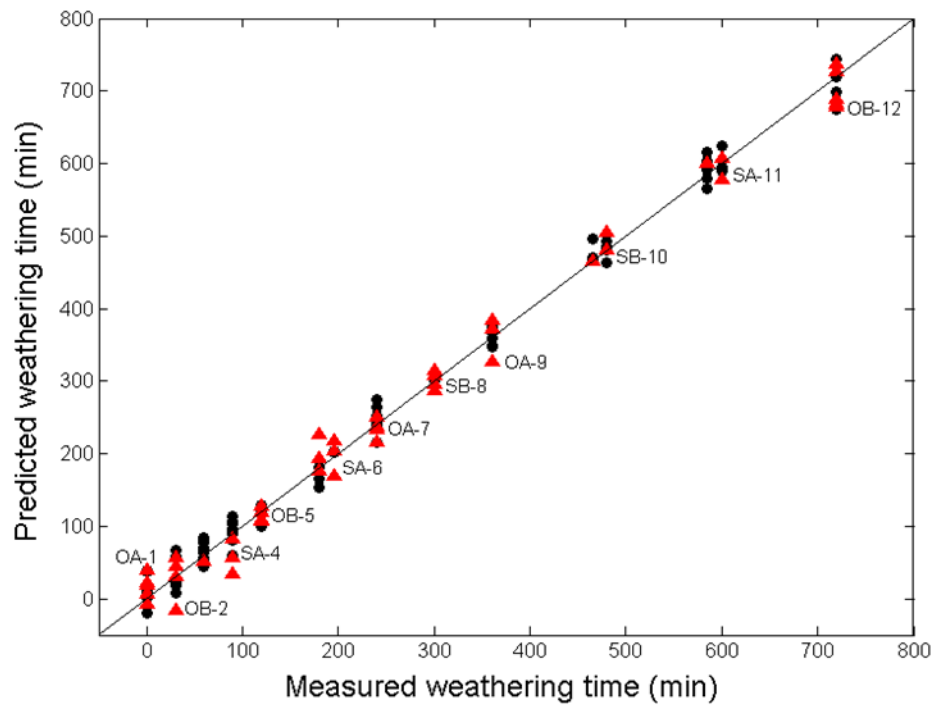


Figure 2-7. LWR calibration for a Class 1 (< 12 h) combined September and October training/test set. Black circles represent the training set and red triangles comprise the test samples. Samples are identified by weathering study, dish and sampling time.

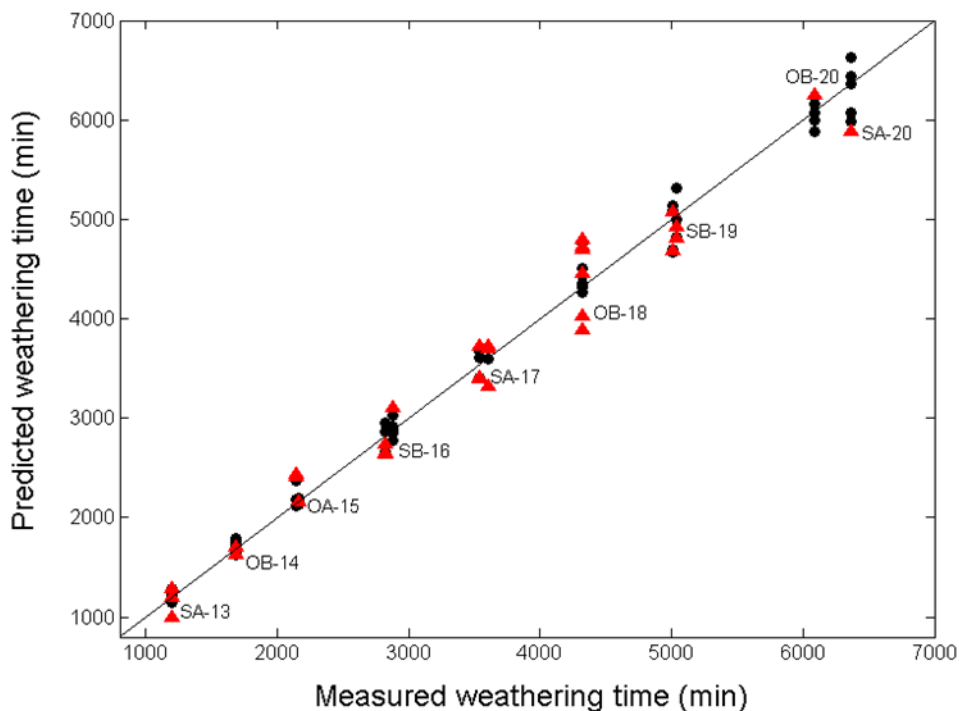


Figure 2-8. LWR calibration for a Class 2 (> 20 h) combined September and October training/test set. Black circles represent the training set and red triangles comprise the test samples. Samples are identified by weathering study, dish and sampling time.

2.4 Conclusions

We have found that estimating the age of a simple hydrocarbon mixture is feasible by first applying a classification model based on PLS-DA to predict whether a sample is relatively fresh or highly weathered. LWR, a nonlinear regression method, can then be used to predict the age of a sample with reasonable accuracy; Class 1 samples (< 12 hours exposure time) estimated to within 40 minutes for all data sets and Class 2 samples (20-100 hours exposure time) to within 4.2 hours.

2.5 References

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3. Using GC×GC-FID profiles to estimate the age of weathered gasoline samples²

3.1 Overview

Comprehensive two-dimensional gas chromatography (GC×GC) is a powerful separation technique used to analyze complex petroleum samples, essentially since its inception [1, 2]. The suitability of this technique, in regards to complex samples, is a result of the large peak capacity that it provides, as well as sensitivity due to refocusing in the second dimension [3, 4]. Moreover, it provides highly ordered chromatograms in which structurally related compounds group together in patterns, facilitating characterization of a sample.

Predicting the amount of time that a petroleum mixture has been exposed to weathering effects has applications in areas of environmental and forensic investigations, such as aiding in determining the cause and intent of a fire. Most research on hydrocarbon weathering has focused on forensic oil spill identification, but to date, few studies have looked at estimating the exposure time of weathered petroleum. The few studies aimed at estimating the age of petroleum contamination have already proven important in litigation due to the high costs associated with spill clean-up. Oukijk [5] estimated the age of heating-oil leaks from underground storage tanks with an error of ± 2 years.

² A version of this chapter is currently in press as an invited paper: B. Zorzetti and J. Harynuk, *Using GC×GC-FID profiles to estimate the age of weathered gasoline samples*, Anal Bioanal Chem.

Similarly, Christensen and Larsen [6] studied degradation ratios between alkanes and isoprenoids from which they could estimate the age of diesel oil spills in a subsurface soil environment with an error ± 2 years for oil exposed between 5-20 years. In this chapter I build upon the work presented in Chapter 2 and apply a hierarchical chemometric approach to the interpretation of GC \times GC chromatographic profiles of weathered gasoline samples to estimate their age.

3.2 Experimental

3.2.1 *Materials and reagents*

Weathering studies were conducted on 87-octane gasoline (four vendors) and 89-octane gasoline (three vendors) collected throughout Edmonton, Alberta. For each gasoline, three 50 mL aliquots were poured into three circular Pyrex[®] dishes (80 \times 40 mm) and placed on a single shelf in the evaporation chamber (labeled dishes A, B & C). Approximately 1 mL of sample was collected from each dish at the designated time using a Pasteur pipette, then stored at -4 °C in sealed 1.8 mL GC sample vials. Temperature was monitored with six evenly spaced thermocouples. Since each gasoline was weathered in triplicate and only six dishes could be placed on the shelf at a time (ie. two gasolines weathered at a time), all seven gasolines were weathered over four separate studies in which the chamber was held at 25.1 ± 0.2 °C, 25.0 ± 0.2 °C, 24.9 ± 0.3 °C and 25.2 ± 0.3 °C respectively. Clean air was passed through

the chamber at a constant flow rate of $11.8 \text{ L}\cdot\text{min}^{-1}$ (16 chamber volumes per hour) for all studies.

Samples of weathered gasoline were collected at varying times during the course of each four-day weathering study. Samples were collected every half-hour during the first two hours of weathering, followed by hourly increments until six hours (total time) had elapsed. This was followed by two-hour increments until 12 hours had elapsed. At this time, eight-hour increments were implemented until 36 hours had elapsed, then twelve-hour intervals until 84 hours had elapsed. Samples were collected until each dish was evaporated to dryness, resulting in a total of 18 to 19 samples collected from each dish (depending on the speed of evaporation). Prior to analysis, weathered samples were brought to room temperature and diluted 100× using pentane (Fisher Scientific, Ottawa, ON) containing chlorocyclohexane (Eastman Chemical Co., Kingsport, TN), p-fluorotoluene (Sigma-Aldrich, Oakville, ON) and 2-fluorobiphenyl (K & K laboratories, New York, NY) as internal standards at concentrations of $0.1 \mu\text{L}\cdot\text{mL}^{-1}$ each.

3.2.2 GC×GC analysis

GC×GC analysis was conducted with an Agilent 7890A gas chromatograph (Agilent Technologies, Mississauga, ON) equipped with a split/splitless injector and flame ionization detector (FID). The primary column was a $15 \text{ m}\times 0.1 \text{ mm}\times 0.1 \mu\text{m}$ Equity-5 (Supelco, Oakville, ON) and the secondary

column was a 3 m×0.25 mm×0.15 μm Innowax (Agilent Technologies). The two columns were interfaced using an Agilent G3486A capillary flow technology (CFT) modulator (Agilent Technologies) operated with a 1.5 s modulation period (1.4 s fill time and 0.1 s flush time). Hydrogen carrier gas was set at a constant flow of 0.2 mL·min⁻¹ in the primary column and 20.4 mL·min⁻¹ in the secondary column. The total run time was 31.4 minutes with an oven program of 32 °C (hold 3 min) to 66 °C at 4 °C·min⁻¹, ramp to 120 °C at 8 °C·min⁻¹, ramp to 140 °C at 10 °C·min⁻¹, with a final ramp of 12 °C·min⁻¹ to 250 °C (hold 2 min). No secondary oven was used. The inlet was held at 250 °C, and operated in split mode with a 1 μL injection at a 100:1 split ratio. The FID was operated at 250 °C and 200 Hz.

3.2.3 Data analysis

Raw chromatographic data were exported from ChemStation (Agilent Technologies) as .CSV files. A lab-written MATLAB (The MathWorks[®], Natick, MA) script (Appendix B) was used to convert the data into a format suitable to be input into ChromaTOF[®] (v. 4.32; Leco, St. Joseph, MI) which was used for peak integration and template classification. Data were collated into spreadsheets and analyzed using PLS Toolbox (v. 6.0.1; Eigenvector Research Inc., Wenatchee, WA).

3.3 Results and Discussion

All samples were analyzed in triplicate by GC×GC-FID, resulting in approximately fifty-seven data points from each dish and approximately 170 per individual gasoline (depending on evaporation rate). Before applying the chemometric models, peaks in each chromatogram were allocated to one of thirty-six categories by overlay of a classification template created using ChromaTOF[®] (Leco) as shown in

Figure 3-1. The groups were chosen to facilitate data analysis by reducing the number of variables, while providing sufficient information for model calculation. The number, location and size of categories were chosen through trial-and-error, as well as being loosely based on prior knowledge acquired from running a simple hydrocarbon mixture containing alkanes and aromatics. The peaks assigned to each category were summed together, creating thirty-six variables for each sample; each category was then normalized (to account for variations in GC injection volume) to one of three IS: chlorocyclohexane for all alkane/alkene groups, p-fluorotoluene for all mono-aromatic groups and 2-fluorobiphenyl for di- and tri-aromatic groups. Raw data are tabulated in Appendix C.

The retention coordinates of the peaks were verified for stability to ensure correct assignment by the template method. Compared to cryogenic modulation devices, pneumatic modulation devices such as the one used in this

study have the disadvantages of requiring relatively short modulation periods and have limited flexibility for adjusting operating conditions without changing the column set. However, they operate without need for added cryogen and avoid retention problems that can arise in cryogenic modulators due to slight variations in heating and cooling times of trapping zones from fluctuations in cryogen delivery and frost build-up on capillaries. Thus there is less concern with analyte peaks shifting into or out of template windows and being misclassified with pneumatic modulation than with cryogenic modulation. Table 3-1 lists the average, minimum and maximum recorded values for the first- and second-dimension retention times for the internal standards across all 1152 samples. Moreover, Figure 3-2 shows a box plot for the second-dimension retention times, clearly demonstrating their reproducibility. A Grubb's test was performed and three outliers were identified in the second-dimension (not shown in the box-plot) at a 95% confidence level. These three outliers are found only for the first IS, however their retention time shifts were less than 100 milliseconds and still fit well within the template categories. Careful manual inspection of these three chromatograms showed that no peaks were misclassified.

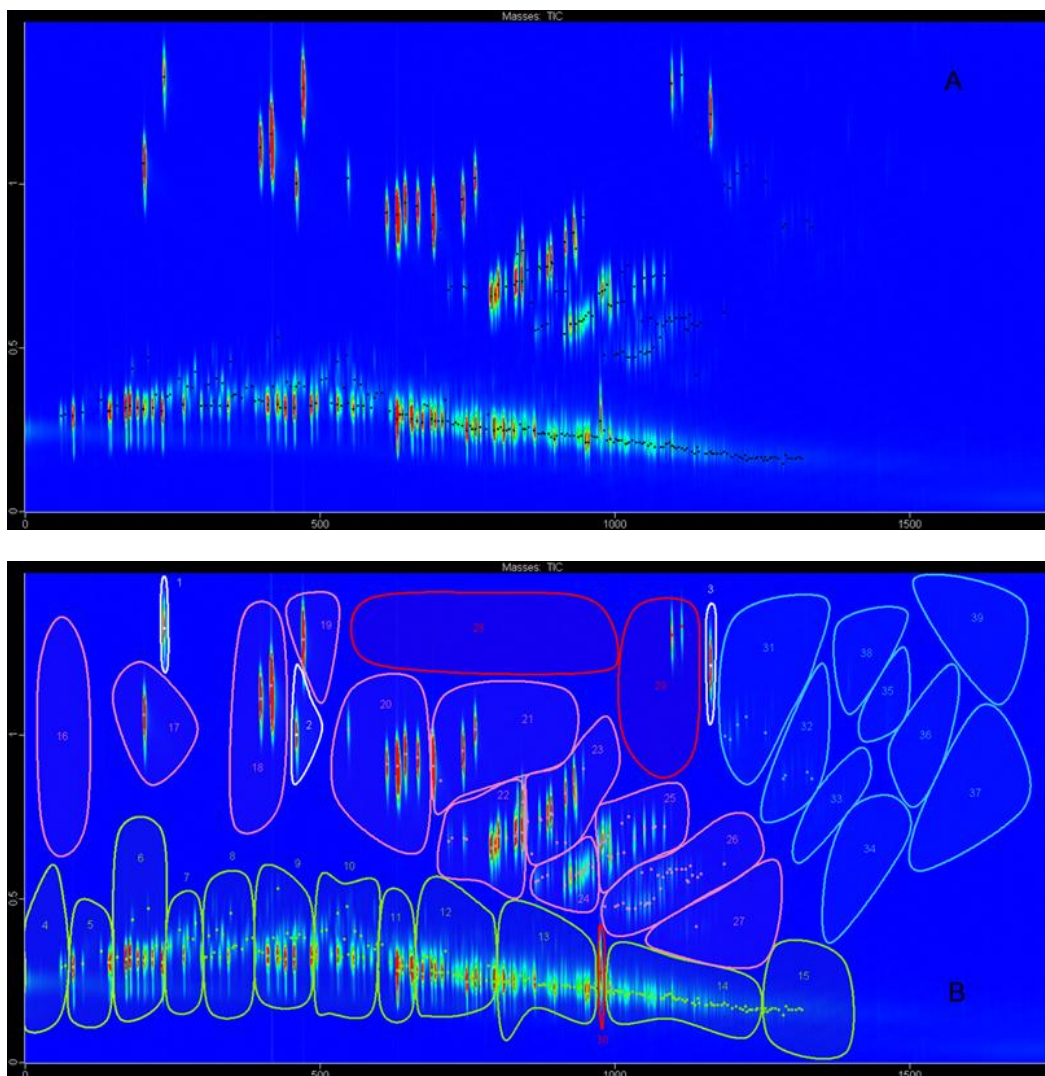


Figure 3-1. GCxGC chromatogram of an 87-octane gasoline sample weathered for approximately 28 hours (A) and a chromatogram containing an overlay for the classification template used to assign each peak to one of thirty-six categories (B). Categories 1 (p-fluorotoluene), 2 (chlorocyclohexane) and 3 (2-fluorobiphenyl) contain the three internal standards used to normalize the categories. Categories 4 through 39 are C6-alkanes, C7-alkanes A, C7-alkanes B, C8-alkanes A, C8-alkanes B, C8-alkanes C, C9-alkanes A, C9-alkanes B, Heavy alkanes A, Heavy alkanes B, Heavy alkanes C, Heavy alkanes D, C6-monoaromatics, C7-monoaromatics, C8-monoaromatics A, C8-monoaromatics B, C9-monoaromatics A, C9-monoaromatics B, C10-monoaromatics A, C10-monoaromatics B, C11/12-monoaromatics A, C11/12-monoaromatics B, Heavy monoaromatics A, Heavy monoaromatics B, Di-aromatics A, Di-aromatics B, Naphthalene, Heavy aromatics A, Heavy aromatics B, Heavy aromatics C, Heavy aromatics D, Heavy aromatics H, Heavy aromatics E, Heavy aromatics F, Heavy aromatics G and Heavy aromatics I, respectively.

Table 3-1. First- and second-dimension retention times (s) for three IS across all gasoline samples ($n = 1152$).

	1t_R (s)			2t_R (s)		
	IS 1	IS 2	IS 3	IS 1	IS 2	IS 3
Mean	236.0	460.0	1161.0	1.352	1.007	1.223
Min	234.0	459.0	1161.0	1.245	0.990	1.205
Max	238.5	462.0	1162.5	1.365	1.015	1.240

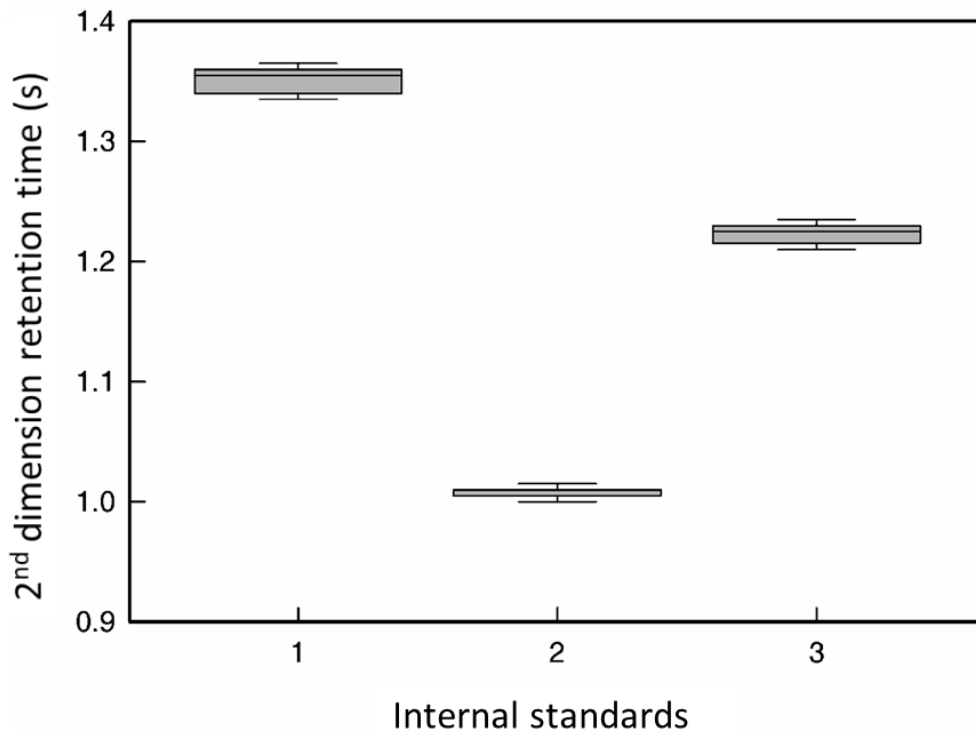


Figure 3-2. Box plot of the second-dimension IS retention times (s). The boundaries of the box indicate the 25th and 75th percentiles; the line within the box marks the median and the whiskers above and below the box indicate the 5th and 95th percentiles.

3.3.1 *Classification of fresh and old gasoline by PLS-DA*

Multiple linear regression (MLR) and PLS were initially investigated for modeling weathering across the entire time range, but the results were unsatisfactory due to the complexity of gasoline's weathering profile (Figure 3-3). As a result, PLS-DA was used to classify the data into a "fresh" and "old" regime prior to performing regression on these two classes.

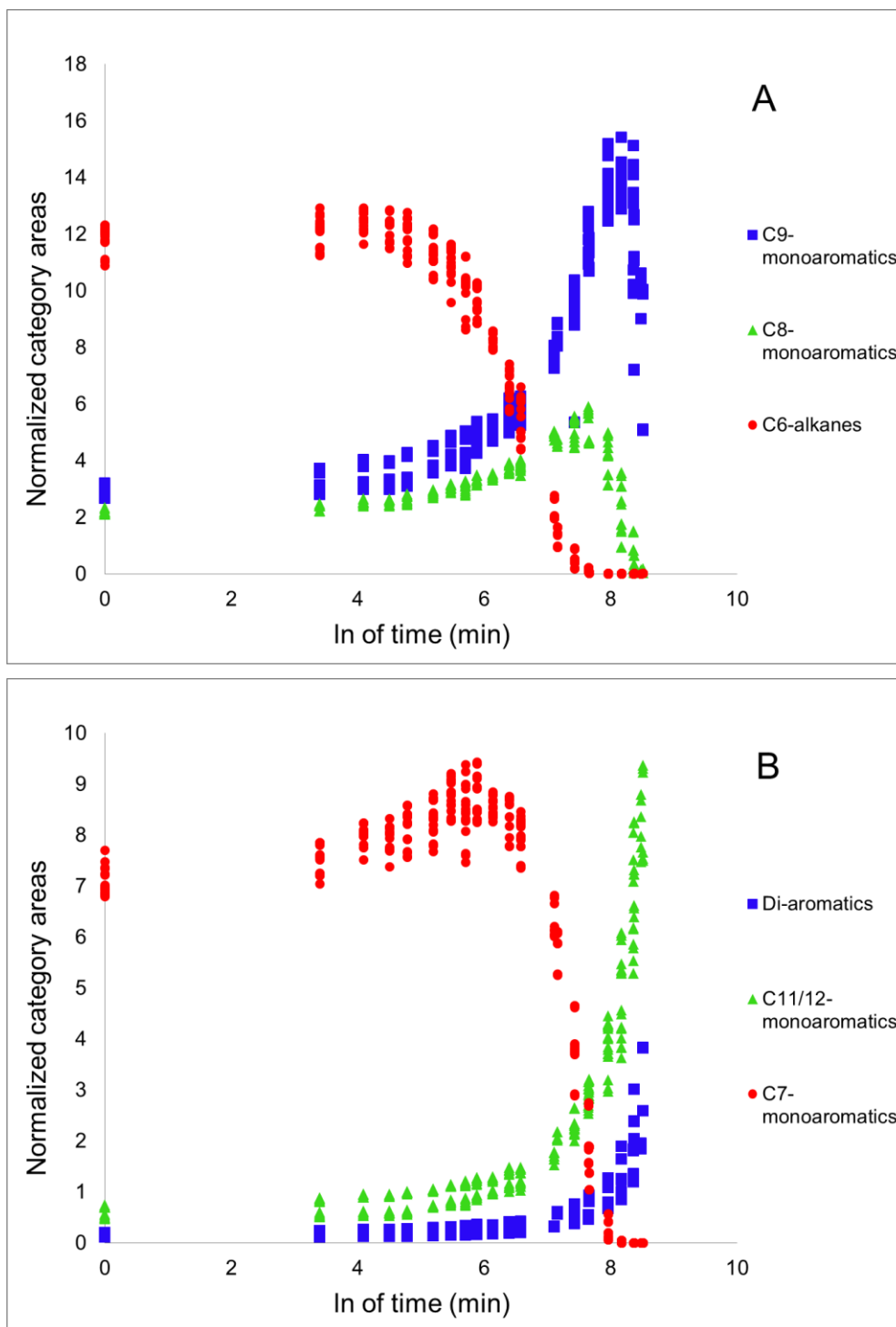


Figure 3-3. Plots of weathering profiles for 87- and 89-octane gasoline. The x-axis represents the natural logarithm of time (min) for each sample taken during weathering and the y-axis represents the normalized category areas. (A) shows the categories believed to consist mostly of C9-monoaromatics, C8-monoaromatics and C6-alkanes; (B) shows the categories believed to consist mostly of Di-aromatics, C11/12-monoaromatics and C7-monoaromatics.

Class 1 was designated for samples weathered 0-12 hours (Samples A, B and C, 1 through 12), and Class 2 was 20-84 hours (Samples A, B and C, 13 through 19). Each replicate measurement taken was treated individually, resulting in a 492 (sample) by 36 (variable) X-block matrix for 89-octane gasolines, a 660 by 36 X-block for 87-octane gasolines and a 1152 by 36 X-block for the combined gasolines. The corresponding class data were assigned to the Y-block. Three different training/test sets were created from these original data matrices by randomly removing one third of the samples to use for model validation (test set). For example, of the 492 samples of 89-octane gasoline, 328 were randomly chosen to form the training set and 164 were chosen as a test set. Similarly, from the 660 samples of 87-octane gasoline, two-thirds formed the training set and one-third formed the test set. The data were preprocessed by autoscaling, which gives all variables equal standing during model calculation, and cross-validated using random subsets. Training sets for the individual and combined octanes were optimized with four to six LVs. The models for the individual octanes all successfully separated the classes and assigned the test samples correctly. For the combined data set, a small number of test or training samples (1%) were misclassified. The same four 87-octane Class 1 samples fell just over the threshold into Class 2 regardless of whether they were training or test samples (Figure 3-4).

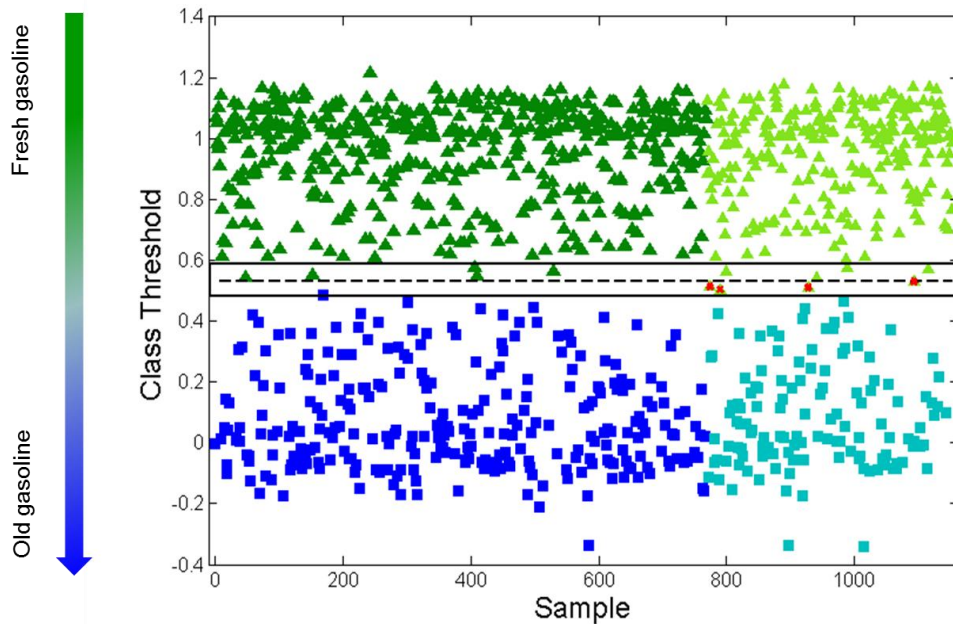


Figure 3-4. PLS-DA of a combined 87- and 89-octane training/test set shows the division between classes. The dark green triangles represent all Class 1 training samples while the light green triangles are the Class 1 test set. The dark blue squares represent Class 2 training samples and light blue squares are the Class 2 test samples. The samples highlighted in red are the misclassified test samples representing 1 % of the total test set. Due to their proximity to the y-threshold (dashed line), a buffer zone was created (solid lines) and samples found within that zone were treated as both Class 1 and Class 2 samples with the final class assignment made on the basis of their Hotelling and Q-residuals. All samples found within the buffer zone had a RMSEP of only 36 minutes when treated as Class 1, but a RMSEP of over 5 hours when treated as Class 2.

It should be noted that the misclassified samples fall so near to the threshold because they were sampled during hour-twelve of the weathering study. In fact, all the samples in the PLS-DA plot show a trend. The most lightly weathered samples fall at the top end of the plot and become more aged as they approach the threshold, with the most weathered samples found at the bottom of the plot. Therefore, even before knowing those samples were misclassified,

they were suspect due to their proximity to the y -threshold, and as a result, these samples were analyzed using both class regression methods to determine which class they most resembled. When treated as members of Class 1, a RMSEP (Equation 2-7) of 36 minutes was observed, with Q-residuals <1 (95% confidence interval at 138) and Hotelling values <13 (95% confidence interval at 10). When membership in Class 2 was assumed, a RMSEP of over 5 hours was observed with Q-residuals of >900 (95% confidence interval at 175) and Hotelling values of 1×10^9 (95% confidence interval at 10). These prediction errors combined with Hotelling and Q-residual values above the 95% confidence interval indicated that these samples were more likely members of Class 1. As no Class 2 samples projected near the threshold of the PLS-DA model, fifty known Class 2 samples were chosen at random and predicted using both class models. The RMSEP for these samples ranged from 18-28 hours when Class 1 models were used, with Q-residuals of >1000 (95% confidence interval at 134) and Hotelling values of 7×10^8 (95% confidence interval at 10). When Class 2 models were used, the RMSEP was 4-5 hours with Hotelling and Q-residuals that were clearly indicative that the samples belong to Class 2. These results indicate that samples falling very near the threshold, regardless of which side they fall, should be treated as belonging to either class, then the final decision on class membership made on the basis of how well the samples fit within the regression models for each class. The success of all training/test sets indicate that this PLS-DA-based approach is

capable of separating weathered classes whose individual samples originate from different octane ratings, as well as different vendors.

3.3.2 Evaluation of PLS, PolyPLS and LWR for predicting weathering times

From the original 492 by 36 X-block of 89-octane gasolines used for PLS-DA, Class 1 samples (<12 hours exposure) reduced to a 321-sample matrix, the 660 by 36 X-block matrix for the 87-octane samples reduced to a 426-sample matrix and the 1152 combined octane samples reduced to a 747-sample matrix. Class 2 (>20 hours exposure) data sets reduced to a 171-sample matrix for the 89-octane samples, a 234-sample matrix for 87-octane samples and a 405-sample matrix for the combined octanes. From each matrix, two-thirds of the samples were randomly chosen to form a training set for model calculation and the remaining samples formed a test set for model validation. This process was repeated to produce three different training/test sets for each matrix on which to build/validate a model. The corresponding time data were assigned to the Y-block. The X and Y matrices were preprocessed by autoscaling. Cross-validation was used to determine the optimal number of LVs by dividing the X-block into ten random subsets. Each subset cycled through once as the test set; the process of random subset cross-validation iterated through five cycles.

The results for all training/test sets were combined to provide a RMSEP range for each regression method as shown in Table 3-2. In general, we see a

positive effect on most Class 2 models with a reduction in overall prediction error and a narrowing of the RMSEP range when the number of samples used to calculate the models is increased by combining the 87- and 89-octane samples. A linear PLS model appears to more accurately predict Class 1 and Class 2 data than a second-order polynomial model, except in the case of Class 2 87-octane samples which respond more accurately to a second-order polynomial. We find that model performance is hindered when a third-order polynomial is used due to overfitting of the training set. Ultimately, we find that LWR outperforms both PLS and PolyPLS regression methods, which is made apparent with the noticeably smaller and narrower RMSEP for both classes.

Table 3-2. RMSEP for all regression methods.

	Class 1 (min)				Class 2 (h)			
	PLS	LWR	PolyPLS (2 nd)	PolyPLS (3 rd)	PLS	LWR	PolyPLS (2 nd)	PolyPLS (3 rd)
87 Octane	39-40	24	37-43	37-49	5.5-6.2	4.3-5.0	5.6-6.0	5.7-6.8
89 Octane	30-33	21-24	32-40	37-40	4.5-5.2	3.7-4.5	4.4-5.5	4.6-6.3
Combined	38-42	24-26	42-49	50-55	5.6-5.8	4.7-5.1	5.4-5.8	5.3-6.2

3.3.3 *Blind experimental validation of the modeling approach*

As a final test of this approach, a blind experiment was run using 87- and 89-octane gasoline samples from the same vendors used in the calibration.

Samples of gasoline were weathered at approximately 25 °C and sampled at random by another member of our research group who recorded the sampling times, but did not divulge the information until after the data were modeled. The samples were analyzed as previously described in the Section 3.2, and the chemometric models applied using the calibration data from the combined 87- and 89-octane data. Samples weathered for fifteen hours or less were assigned to Class 1 using PLS-DA, and samples weathered for over fifteen hours were clearly categorized as Class 2. One sample fell within the buffer zone straddling the class threshold; this sample was treated as both Class 1 and 2. Based on the Hotelling and Q-residual values for the sample in the two models, it was deemed to be more likely from Class 1, and later found to be predicted to within twelve minutes of the true time, whereas the residual was larger than 6 hours when treated as Class 2. The overall RMSEP for the blind controls was 38 minutes for Class 1 and 4.6 hours for Class 2 (Figure 3-5). The measured and predicted times (min) for each weathered blind control sample are presented in Table 3-3. Sample identification numbers containing an A or B designation indicate those samples weathered in duplicate (i.e., dish A or dish B). Samples were only weathered in duplicate when sufficient volumes of the original gasoline samples were available. Class 2 samples were estimated slightly more accurately than expected from the original models, while the errors in the original Class 1 predictions were slightly optimistic. Overall, the prediction error of the blind controls suggest that the predictive models created using PLS-DA and LWR may

be viable in predicting real-world samples once the models have been expanded to include other factors involved in hydrocarbon weathering such as temperature and air flow.

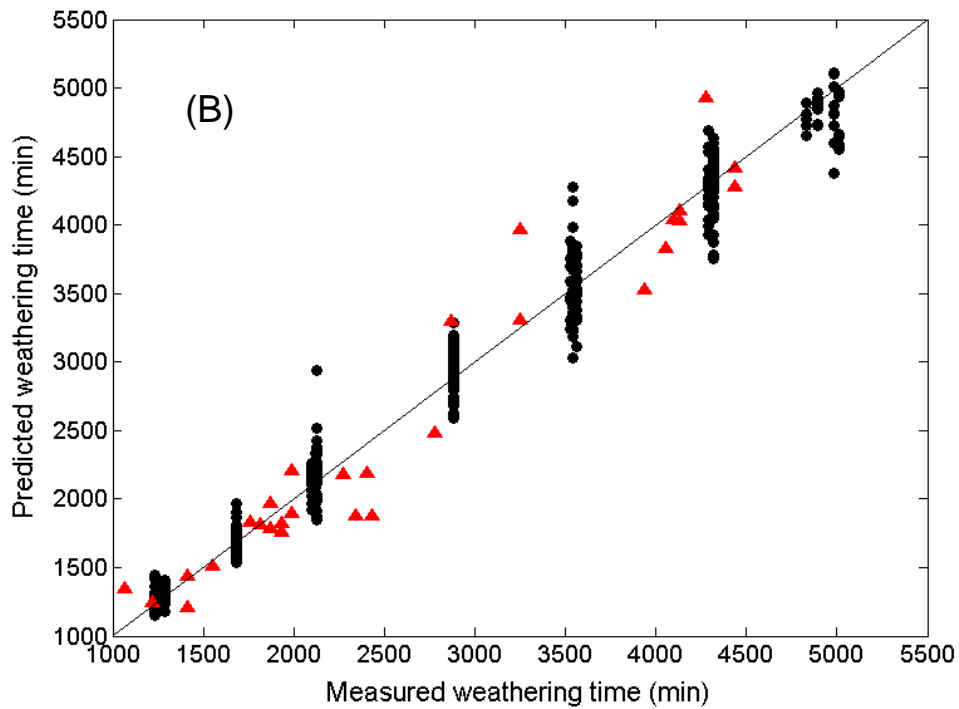
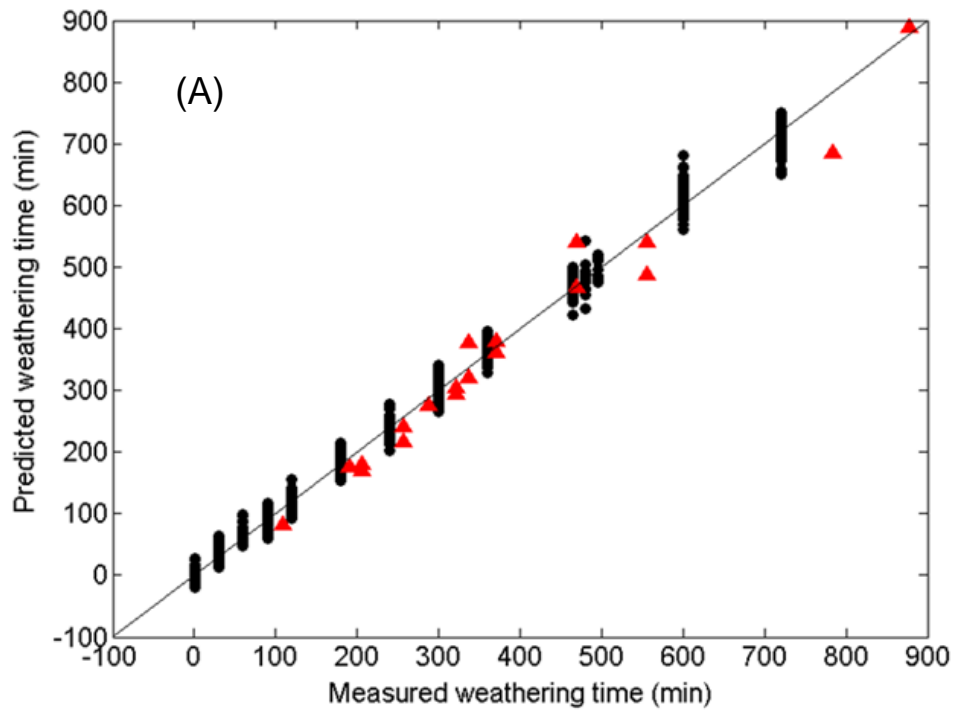


Figure 3-5. LWR calibration of expected vs. predicted weathering times for the Class 1 blind controls (A) and Class 2 blind controls (B). The circles represent calibration data and the triangles the blind control test.

Table 3-3. Measured vs. predicted weathering time (min) for blind control samples.

Class 1			Class 2		
Sample ID#	Measured time (min)	Predicted time (min)	Sample ID#	Measured time (min)	Predicted time (min)
536	109	82	657	1067	1341
427	190	176	384	1221	1244
162A	206	169	102A	1416	1211
162B	206	180	102B	1416	1435
375A	257	216	864A	1551	1513
375B	257	242	864B	1551	1505
218	288	276	522	1758	1826
712A	321	294	412	1817	1812
712B	321	305	813A	1871	1781
112A	337	321	813B	1871	1968
112B	337	377	273A	1936	1752
600A	371	362	273B	1936	1818
600B	371	380	162A	1990	1895
442A	469	468	162B	1990	2201
442B	469	540	560	2272	2173
311A	556	488	617	2344	1878
311B	556	541	317	2407	2186
361	784	684	722	2433	1872
111	878	888	430	2780	2481

	751	2868	3294
	780A	3247	3309
	780B	3247	3966
	227	3938	3528
	516	4056	3829
	109	4093	4034
	966	4128	4027
	737	4128	4106
	921	4274	4924
	260A	4436	4276
	260B	4436	4417

3.4 Conclusions

Analysis with GC×GC provides ample data with which to monitor the weathering behavior of complex petroleum mixtures such as gasoline. By grouping the hundreds of peaks detected in each chromatogram into thirty-six categories, then using a hierarchical application of multivariate techniques, we have determined that estimating the age of a weathered gasoline sample is feasible. Classification using PLS-DA is successful in predicting whether a sample is relatively fresh or highly weathered. A LWR method can then be used to predict the age of a sample with reasonable accuracy; Class 1 samples (< 12 hours exposure time) estimated to within thirty minutes for all data sets (38 min

for blind controls) and Class 2 samples (> 20 hours exposure time) to within five hours. This work indicates that the ability to predict the age of other complex petroleum mixtures may also be feasible, though the classification template will likely need to be adjusted for each new mixture.

3.5 References

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4. Chapter Four

4.1 General Conclusions

The purpose of this research was to determine the feasibility of predicting the age of weathered hydrocarbon mixtures for application in environmental and forensic fields. Although our models remained simple with a constant temperature and airflow throughout the weathering studies, the results appear promising for more complex systems. Two-dimensional gas chromatography provides ample information on weathered samples; even though we chose to simplify the data by applying a classification template to reduce our sample variables from hundreds of peaks to thirty-six categories, using the individual peaks from each chromatogram can provide the information necessary to model more complex weathering systems.

Returning to the original purpose of this research, we believe that our models have the potential for real-world applicability. Even though we controlled temperature and airflow during the gasoline weathering studies, our models reflect that enough information is available to pull patterns from the weathering profiles to first assign gasoline samples to a 0-12 hour time range or a 20-84 hour time range. From there, the use of nonlinear regression further narrows down the prediction range to within 30 minutes for the lightly weathered samples and 5 hours for the highly weathered samples. If future models are capable of

predicting the age of ignitable liquids found at a fire scene to within these ranges, forensic investigators will have a useful tool with which to establish the intent of a fire.

4.2 Future Work

One complication which arose early in this research was the divergent weathering profiles of samples evaporated on different shelves in the weathering chamber. Even though the temperature of the shelves varied by less than one degree, that difference, likely along with slight differences in airflow, created weathered data more complex than desired for an initial study. Our focus with this research was to keep the experimental conditions steady and simple in order to establish the feasibility of predicting petroleum mixtures. However, for this research to have any hope of real world application, further study is required to extend our models to more complex weathering systems by altering the weathering conditions (temperature, airflow and humidity), varying the substrates on which the pools are placed for weathering studies (carpet mixtures, cement, wood, etc.), and investigating different petroleum mixtures (paint thinner, kerosene, etc.).

It may also be possible to further extend our time range for the weathering studies. Though samples were collected from the weathering dishes until all liquid had evaporated, a residue remained in the dishes. In future studies, it may be possible to swab this residue and rinse the swab with solvent

to extract the remaining residue. Furthermore, although the multivariate techniques chosen for the gasoline data were sufficient for our predictions, no doubt future models (encompassing variations in weathering conditions) will require investigation into more complex preprocessing and chemometric techniques to deal with the increasing complexity of the data.

5. Appendices

Appendix A

Fraction of each compound in a weathered nine-compound mixture (area ratio of each compound divided by the total area ratio). Samples weathered in September are labeled SA and SB; October samples are OA and OB.

Sample #	Benzene	2,2,4-trimethylpentane	Heptane	Toluene	m-Xylene	Nonane	Decane	1,2,3,5-tetramethylbenzene	Naphthalene	Weathering time (min)
OA-1	0.0759	0.0704	0.0579	0.1153	0.1421	0.0928	0.1118	0.2080	0.1008	1
OA-1	0.0730	0.0710	0.0577	0.1144	0.1431	0.0942	0.1128	0.2090	0.0997	1
OA-1	0.0770	0.0716	0.0591	0.1157	0.1420	0.0949	0.1123	0.2057	0.0971	1
OA-10	0.0329	0.0518	0.0437	0.0972	0.1451	0.1023	0.1315	0.2463	0.1195	465
OA-10	0.0387	0.0580	0.0480	0.1072	0.1523	0.1032	0.1248	0.2287	0.1114	465
OA-10	0.0397	0.0585	0.0494	0.1086	0.1534	0.1038	0.1247	0.2264	0.1083	465
OA-11	0.0306	0.0522	0.0444	0.1025	0.1539	0.1053	0.1287	0.2381	0.1158	585
OA-11	0.0294	0.0530	0.0447	0.1022	0.1553	0.1067	0.1298	0.2372	0.1136	585
OA-11	0.0261	0.0485	0.0406	0.0938	0.1498	0.1062	0.1332	0.2508	0.1210	585
OA-12	0.0207	0.0436	0.0372	0.0894	0.1477	0.1045	0.1349	0.2614	0.1293	720
OA-12	0.0202	0.0446	0.0377	0.0917	0.1516	0.1079	0.1366	0.2549	0.1243	720
OA-12	0.0218	0.0471	0.0395	0.0967	0.1555	0.1078	0.1337	0.2482	0.1198	720
OA-13	0.0065	0.0306	0.0269	0.0772	0.1600	0.1167	0.1474	0.2719	0.1304	1200
OA-13	0.0067	0.0311	0.0271	0.0776	0.1609	0.1172	0.1472	0.2708	0.1294	1200
OA-13	0.0062	0.0297	0.0261	0.0745	0.1564	0.1150	0.1475	0.2772	0.1340	1200
OA-14	0.0012	0.0153	0.0139	0.0500	0.1461	0.1154	0.1587	0.3101	0.1520	1680
OA-14	0.0014	0.0161	0.0146	0.0522	0.1506	0.1170	0.1579	0.3034	0.1498	1680

Sample #	Benzene	2,2,4-trimethylpentane	Heptane	Toluene	m-Xylene	Nonane	Decane	1,2,3,5-tetramethylbenzene	Naphthalene	Weathering time (min)
OA-14	0.0014	0.0155	0.0139	0.0505	0.1436	0.1119	0.1576	0.3118	0.1556	1680
OA-15	0	0.0062	0.0060	0.0299	0.1354	0.1154	0.1675	0.3332	0.1659	2145
OA-15	0	0.0063	0.0060	0.0308	0.1373	0.1171	0.1683	0.3309	0.1634	2145
OA-15	0	0.0069	0.0067	0.0338	0.1440	0.1202	0.1687	0.3237	0.1573	2145
OA-16	0	0	0	0.0141	0.1192	0.1138	0.1781	0.3562	0.1753	2820
OA-16	0	0	0	0.0126	0.1105	0.1087	0.1775	0.3654	0.1814	2820
OA-16	0	0	0	0.0143	0.1179	0.1126	0.1778	0.3572	0.1770	2820
OA-17	0	0	0	0.0032	0.0898	0.1052	0.1855	0.3814	0.1888	3540
OA-17	0	0	0	0.0033	0.0921	0.1078	0.1883	0.3792	0.1841	3540
OA-17	0	0	0	0.0034	0.0914	0.1062	0.1849	0.3797	0.1882	3540
OA-18	0	0	0	0	0.0473	0.0797	0.1873	0.4207	0.2132	4320
OA-18	0	0	0	0	0.0505	0.0839	0.1900	0.4147	0.2094	4320
OA-18	0	0	0	0	0.0536	0.0873	0.1933	0.4134	0.2023	4320
OA-19	0	0	0	0	0.0273	0.0606	0.1788	0.4465	0.2325	5010
OA-19	0	0	0	0	0.0317	0.0687	0.1889	0.4374	0.2198	5010
OA-19	0	0	0	0	0.0260	0.0593	0.1803	0.4478	0.2324	5010
OA-2	0.0709	0.0687	0.0569	0.1134	0.1415	0.0948	0.1139	0.2125	0.1022	30
OA-2	0.0746	0.0704	0.0578	0.1147	0.1414	0.0942	0.1124	0.2093	0.1007	30
OA-2	0.0705	0.0687	0.0565	0.1126	0.1403	0.0941	0.1149	0.2137	0.1032	30
OA-20	0	0	0	0	0.0066	0.0314	0.1722	0.4847	0.2467	6090
OA-20	0	0	0	0	0.0066	0.0310	0.1725	0.4808	0.2495	6090
OA-20	0	0	0	0	0.0053	0.0269	0.1637	0.4843	0.2594	6090
OA-21	0	0	0	0	0	0.0034	0.1102	0.5331	0.2910	7500
OA-21	0	0	0	0	0	0.0034	0.1109	0.5298	0.2931	7500
OA-21	0	0	0	0	0	0.0033	0.1105	0.5321	0.2920	7500

Sample #	Benzene	2,2,4-trimethylpentane	Heptane	Toluene	m-Xylene	Nonane	Decane	1,2,3,5-tetramethylbenzene	Naphthalene	Weathering time (min)
OA-3	0.0729	0.0695	0.0569	0.1141	0.1415	0.0943	0.1142	0.2116	0.1005	60
OA-3	0.0650	0.0636	0.0515	0.1042	0.1340	0.0912	0.1171	0.2323	0.1139	60
OA-3	0.0675	0.0679	0.0560	0.1109	0.1411	0.0946	0.1140	0.2180	0.1040	60
OA-4	0.0638	0.0660	0.0544	0.1084	0.1419	0.0957	0.1174	0.2206	0.1060	90
OA-4	0.0621	0.0642	0.0534	0.1076	0.1398	0.0945	0.1176	0.2248	0.1091	90
OA-4	0.0659	0.0685	0.0565	0.1134	0.1438	0.0965	0.1156	0.2126	0.1018	90
OA-5	0.0657	0.0692	0.0568	0.1147	0.1459	0.0975	0.1161	0.2095	0.0998	120
OA-5	0.0617	0.0644	0.0534	0.1081	0.1422	0.0971	0.1190	0.2211	0.1061	120
OA-5	0.0645	0.0672	0.0558	0.1137	0.1438	0.0956	0.1156	0.2144	0.1039	120
OA-6	0.0561	0.0643	0.0534	0.1090	0.1440	0.0983	0.1189	0.2227	0.1071	195
OA-6	0.0601	0.0674	0.0564	0.1143	0.1489	0.0993	0.1171	0.2112	0.1003	195
OA-6	0.0583	0.0661	0.0545	0.1117	0.1445	0.0984	0.1188	0.2173	0.1049	195
OA-7	0.0578	0.0658	0.0548	0.1138	0.1491	0.0987	0.1182	0.2148	0.1017	240
OA-7	0.0577	0.0656	0.0546	0.1132	0.1480	0.0986	0.1176	0.2163	0.1026	240
OA-7	0.0558	0.0645	0.0533	0.1111	0.1456	0.0978	0.1181	0.2206	0.1069	240
OA-8	0.0522	0.0640	0.0531	0.1121	0.1503	0.1006	0.1200	0.2186	0.1033	300
OA-8	0.0500	0.0609	0.0506	0.1072	0.1447	0.0985	0.1214	0.2288	0.1107	300
OA-8	0.0420	0.0547	0.0455	0.0976	0.1412	0.0986	0.1272	0.2440	0.1197	300
OA-9	0.0459	0.0595	0.0495	0.1062	0.1470	0.1006	0.1233	0.2294	0.1110	360
OA-9	0.0435	0.0575	0.0487	0.1044	0.1475	0.1015	0.1249	0.2321	0.1123	360
OA-9	0.0450	0.0600	0.0503	0.1078	0.1490	0.1016	0.1238	0.2271	0.1085	360
OB-1	0.0632	0.0638	0.0528	0.1046	0.1372	0.0939	0.1182	0.2273	0.1118	1
OB-1	0.0771	0.0733	0.0596	0.1186	0.1430	0.0948	0.1114	0.2023	0.0964	1
OB-1	0.0810	0.0736	0.0603	0.1186	0.1436	0.0935	0.1103	0.2000	0.0956	1
OB-10	0.0442	0.0610	0.0507	0.1114	0.1510	0.1034	0.1232	0.2223	0.1064	465

Sample #	Benzene	2,2,4-trimethylpentane	Heptane	Toluene	m-Xylene	Nonane	Decane	1,2,3,5-tetramethylbenzene	Naphthalene	Weathering time (min)
OB-10	0.0378	0.0559	0.0469	0.1034	0.1481	0.1022	0.1265	0.2364	0.1150	465
OB-10	0.0393	0.0600	0.0501	0.1085	0.1525	0.1048	0.1255	0.2260	0.1072	465
OB-11	0.0299	0.0500	0.0422	0.0964	0.1469	0.1025	0.1312	0.2490	0.1222	585
OB-11	0.0349	0.0556	0.0470	0.1074	0.1548	0.1041	0.1266	0.2308	0.1112	585
OB-11	0.0301	0.0513	0.0436	0.0993	0.1504	0.1043	0.1287	0.2443	0.1194	585
OB-12	0.0270	0.0505	0.0426	0.1005	0.1536	0.1074	0.1306	0.2432	0.1163	720
OB-12	0.0221	0.0451	0.0380	0.0905	0.1464	0.1036	0.1346	0.2609	0.1281	720
OB-12	0.0240	0.0467	0.0394	0.0936	0.1489	0.1047	0.1334	0.2543	0.1246	720
OB-13	0.0077	0.0313	0.0272	0.0760	0.1526	0.1117	0.1458	0.2793	0.1350	1200
OB-13	0.0087	0.0341	0.0298	0.0826	0.1594	0.1149	0.1436	0.2668	0.1282	1200
OB-13	0.0079	0.0311	0.0274	0.0768	0.1520	0.1110	0.1435	0.2787	0.1384	1200
OB-14	0.0022	0.0206	0.0185	0.0628	0.1588	0.1191	0.1530	0.2888	0.1410	1680
OB-14	0.0022	0.0204	0.0184	0.0627	0.1603	0.1204	0.1551	0.2885	0.1381	1680
OB-14	0.0022	0.0202	0.0183	0.0616	0.1576	0.1207	0.1550	0.2897	0.1401	1680
OB-15	0	0.0076	0.0072	0.0315	0.1209	0.1032	0.1602	0.3481	0.1796	2145
OB-15	0	0.0107	0.0100	0.0435	0.1525	0.1220	0.1646	0.3098	0.1495	2145
OB-15	0	0.0109	0.0102	0.0439	0.1533	0.1230	0.1628	0.3096	0.1494	2145
OB-16	0	0.0029	0.0029	0.0202	0.1279	0.1162	0.1727	0.3457	0.1696	2820
OB-16	0	0.0032	0.0032	0.0225	0.1377	0.1216	0.1752	0.3356	0.1613	2820
OB-16	0	0.0031	0.0031	0.0213	0.1339	0.1193	0.1748	0.3390	0.1647	2820
OB-17	0	0	0	0.0068	0.1074	0.1126	0.1836	0.3662	0.1792	3540
OB-17	0	0	0	0.0068	0.1084	0.1141	0.1841	0.3662	0.1765	3540
OB-17	0	0	0	0.0067	0.1057	0.1113	0.1828	0.3691	0.1801	3540
OB-18	0	0	0	0	0.0780	0.0989	0.1876	0.3928	0.1957	4320
OB-18	0	0	0	0	0.0822	0.1035	0.1899	0.3869	0.1902	4320

Sample #	Benzene	2,2,4-trimethylpentane	Heptane	Toluene	m-Xylene	Nonane	Decane	1,2,3,5-tetramethylbenzene	Naphthalene	Weathering time (min)
OB-18	0	0	0	0	0.0731	0.0951	0.1881	0.3993	0.1969	4320
OB-19	0	0	0	0	0.0527	0.0835	0.1867	0.4169	0.2099	5010
OB-19	0	0	0	0	0.0574	0.0886	0.1892	0.4096	0.2053	5010
OB-19	0	0	0	0	0.0499	0.0799	0.1839	0.4204	0.2141	5010
OB-2	0.0745	0.0714	0.0596	0.1165	0.1435	0.0956	0.1131	0.2046	0.0975	30
OB-2	0.0694	0.0674	0.0560	0.1110	0.1399	0.0955	0.1165	0.2156	0.1033	30
OB-2	0.0774	0.0724	0.0588	0.1159	0.1425	0.0952	0.1122	0.2042	0.0974	30
OB-20	0	0	0	0	0.0206	0.0558	0.1886	0.4522	0.2276	6090
OB-20	0	0	0	0	0.0197	0.0543	0.1850	0.4532	0.2319	6090
OB-20	0	0	0	0	0.0202	0.0552	0.1855	0.4529	0.2305	6090
OB-21	0	0	0	0	0.0021	0.0159	0.1494	0.5038	0.2680	7500
OB-21	0	0	0	0	0.0019	0.0155	0.1498	0.5009	0.2702	7500
OB-21	0	0	0	0	0.0019	0.0159	0.1513	0.5019	0.2677	7500
OB-3	0.0717	0.0721	0.0599	0.1172	0.1444	0.0969	0.1138	0.2031	0.0970	60
OB-3	0.0753	0.0713	0.0596	0.1174	0.1431	0.0955	0.1135	0.2041	0.0971	60
OB-3	0.0691	0.0686	0.0566	0.1116	0.1396	0.0951	0.1165	0.2146	0.1034	60
OB-4	0.0685	0.0682	0.0565	0.1126	0.1409	0.0946	0.1154	0.2148	0.1039	90
OB-4	0.0721	0.0711	0.0585	0.1180	0.1445	0.0959	0.1138	0.2047	0.0976	90
OB-4	0.0592	0.0611	0.0499	0.1015	0.1341	0.0938	0.1204	0.2362	0.1162	90
OB-5	0.0691	0.0705	0.0585	0.1177	0.1451	0.0961	0.1149	0.2058	0.0979	120
OB-5	0.0697	0.0709	0.0583	0.1174	0.1461	0.0974	0.1142	0.2046	0.0973	120
OB-5	0.0657	0.0668	0.0554	0.1117	0.1402	0.0954	0.1168	0.2178	0.1053	120
OB-6	0.0677	0.0699	0.0572	0.1183	0.1471	0.0971	0.1148	0.2057	0.0980	195
OB-6	0.0543	0.0631	0.0521	0.1058	0.1426	0.0994	0.1225	0.2250	0.1090	195
OB-6	0.0654	0.0679	0.0563	0.1157	0.1449	0.0980	0.1164	0.2109	0.1007	195

Sample #	Benzene	2,2,4-trimethylpentane	Heptane	Toluene	m-Xylene	Nonane	Decane	1,2,3,5-tetramethylbenzene	Naphthalene	Weathering time (min)
OB-7	0.0590	0.0669	0.0553	0.1145	0.1482	0.0994	0.1181	0.2124	0.1009	240
OB-7	0.0547	0.0633	0.0530	0.1096	0.1468	0.0995	0.1205	0.2197	0.1069	240
OB-7	0.0523	0.0619	0.0507	0.1058	0.1436	0.0994	0.1226	0.2268	0.1104	240
OB-8	0.0494	0.0612	0.0512	0.1080	0.1456	0.0986	0.1208	0.2274	0.1105	300
OB-8	0.0483	0.0599	0.0501	0.1058	0.1450	0.0995	0.1229	0.2294	0.1118	300
OB-8	0.0556	0.0642	0.0535	0.1128	0.1475	0.0990	0.1188	0.2180	0.1048	300
OB-9	0.0529	0.0637	0.0543	0.1141	0.1496	0.1012	0.1197	0.2166	0.1025	360
OB-9	0.0473	0.0615	0.0510	0.1084	0.1455	0.1009	0.1223	0.2268	0.1099	360
OB-9	0.0480	0.0621	0.0520	0.1088	0.1472	0.1004	0.1222	0.2247	0.1086	360
SA-1	0.0862	0.0815	0.0701	0.1213	0.1274	0.1068	0.1307	0.1625	0.0955	1
SA-1	0.0910	0.0828	0.0728	0.1279	0.1325	0.0985	0.1132	0.1683	0.0971	1
SA-1	0.0889	0.0850	0.0724	0.1273	0.1307	0.0988	0.1114	0.1727	0.0977	1
SA-10	0.0430	0.0677	0.0593	0.1170	0.1434	0.1108	0.1300	0.2004	0.1097	480
SA-10	0.0337	0.0562	0.0491	0.0975	0.1318	0.1104	0.1417	0.2248	0.1331	480
SA-10	0.0437	0.0626	0.0558	0.1090	0.1358	0.1171	0.1487	0.1913	0.1148	480
SA-11	0.0354	0.0623	0.0554	0.1123	0.1450	0.1139	0.1340	0.2043	0.1183	600
SA-11	0.0353	0.0624	0.0548	0.1129	0.1454	0.1117	0.1334	0.2066	0.1187	600
SA-11	0.0352	0.0626	0.0554	0.1101	0.1428	0.1233	0.1523	0.1871	0.1104	600
SA-12	0.0296	0.0585	0.0521	0.1112	0.1471	0.1141	0.1359	0.2100	0.1217	720
SA-12	0.0279	0.0591	0.0516	0.1093	0.1482	0.1161	0.1379	0.2110	0.1199	720
SA-12	0.0268	0.0531	0.0478	0.1005	0.1419	0.1240	0.1596	0.2032	0.1200	720
SA-13	0.0109	0.0418	0.0376	0.0935	0.1524	0.1245	0.1510	0.2328	0.1341	1200
SA-13	0.0109	0.0433	0.0379	0.0936	0.1531	0.1263	0.1492	0.2361	0.1308	1200
SA-13	0.0099	0.0377	0.0342	0.0831	0.1424	0.1324	0.1749	0.2256	0.1350	1200
SA-14	0.0024	0.0215	0.0201	0.0622	0.1418	0.1247	0.1680	0.2717	0.1600	1680

Sample #	Benzene	2,2,4-trimethylpentane	Heptane	Toluene	m-Xylene	Nonane	Decane	1,2,3,5-tetramethylbenzene	Naphthalene	Weathering time (min)
SA-14	0.0027	0.0267	0.0239	0.0711	0.1524	0.1326	0.1612	0.2622	0.1456	1680
SA-14	0.0029	0.0237	0.0220	0.0650	0.1434	0.1380	0.1872	0.2446	0.1459	1680
SA-15	0	0.0128	0.0122	0.0467	0.1439	0.1320	0.1748	0.2849	0.1664	2160
SA-15	0	0.0133	0.0126	0.0489	0.1448	0.1305	0.1737	0.2811	0.1678	2160
SA-15	0	0.0131	0.0127	0.0473	0.1427	0.1422	0.1963	0.2599	0.1563	2160
SA-16	0	0.0036	0.0036	0.0218	0.1211	0.1252	0.1895	0.3162	0.1865	2880
SA-16	0	0.0042	0.0042	0.0251	0.1337	0.1339	0.1900	0.3036	0.1749	2880
SA-16	0	0.0040	0.0042	0.0248	0.1291	0.1424	0.2118	0.2815	0.1702	2880
SA-17	0	0	0	0.0094	0.1133	0.1316	0.1984	0.3279	0.1897	3600
SA-17	0	0	0	0.0109	0.1155	0.1294	0.1982	0.3228	0.1899	3600
SA-17	0	0	0	0.0110	0.1121	0.1386	0.2220	0.3007	0.1813	3600
SA-18	0	0	0	0	0.0882	0.1194	0.2058	0.3455	0.2062	4320
SA-18	0	0	0	0	0.0910	0.1196	0.2042	0.3440	0.2043	4320
SA-18	0	0	0	0.0029	0.0794	0.1185	0.2212	0.3339	0.2054	4320
SA-19	0	0	0	0	0.0687	0.1072	0.2092	0.3620	0.2141	5040
SA-19	0	0	0	0	0.0666	0.1071	0.2110	0.3635	0.2157	5040
SA-19	0	0	0	0	0.0652	0.1141	0.2261	0.3432	0.2112	5040
SA-2	0.0877	0.0839	0.0720	0.1255	0.1299	0.1002	0.1113	0.1769	0.0972	30
SA-2	0.0608	0.0701	0.0612	0.1093	0.1310	0.1052	0.1303	0.1963	0.1157	30
SA-2	0.0943	0.0842	0.0729	0.1270	0.1306	0.1069	0.1260	0.1526	0.0883	30
SA-20	0	0	0	0	0.0346	0.0832	0.2114	0.3935	0.2369	6360
SA-20	0	0	0	0	0.0315	0.0791	0.2087	0.4042	0.2384	6360
SA-20	0	0	0	0	0.0355	0.0908	0.2354	0.3693	0.2268	6360
SA-21	0	0	0	0	0.0142	0.0570	0.2059	0.4226	0.2589	7800
SA-21	0	0	0	0	0.0146	0.0571	0.2084	0.4255	0.2509	7800

Sample #	Benzene	2,2,4-trimethylpentane	Heptane	Toluene	m-Xylene	Nonane	Decane	1,2,3,5-tetramethylbenzene	Naphthalene	Weathering time (min)
SA-21	0	0	0	0	0.0163	0.0651	0.2283	0.3970	0.2475	7800
SA-22	0	0	0	0	0.0038	0.0317	0.1911	0.4543	0.2706	9000
SA-22	0	0	0	0	0.0030	0.0318	0.1896	0.4528	0.2762	9000
SA-22	0	0	0	0	0.0052	0.0379	0.2159	0.4267	0.2638	9000
SA-3	0.0851	0.0837	0.0721	0.1262	0.1335	0.1008	0.1164	0.1744	0.0948	60
SA-3	0.0826	0.0841	0.0718	0.1274	0.1326	0.1008	0.1135	0.1742	0.0989	60
SA-3	0.0706	0.0748	0.0646	0.1147	0.1298	0.1113	0.1397	0.1740	0.1011	60
SA-4	0.0777	0.0802	0.0695	0.1242	0.1335	0.1002	0.1172	0.1786	0.1024	90
SA-4	0.0794	0.0818	0.0703	0.1244	0.1336	0.1005	0.1143	0.1791	0.1017	90
SA-4	0.0780	0.0766	0.0659	0.1176	0.1280	0.1088	0.1359	0.1700	0.1004	90
SA-5	0.0902	0.0872	0.0737	0.1299	0.1271	0.0988	0.1105	0.1765	0.0937	120
SA-5	0.0749	0.0791	0.0686	0.1239	0.1332	0.1007	0.1178	0.1798	0.1050	120
SA-5	0.0824	0.0820	0.0704	0.1249	0.1322	0.1110	0.1308	0.1589	0.0909	120
SA-6	0.0726	0.0786	0.0684	0.1240	0.1354	0.1017	0.1193	0.1796	0.1039	180
SA-6	0.0641	0.0735	0.0654	0.1180	0.1334	0.1024	0.1234	0.1894	0.1125	180
SA-6	0.0608	0.0687	0.0603	0.1106	0.1312	0.1123	0.1439	0.1827	0.1088	180
SA-7	0.0610	0.0701	0.0610	0.1145	0.1325	0.1019	0.1261	0.1973	0.1157	240
SA-7	0.0654	0.0767	0.0666	0.1219	0.1346	0.1050	0.1188	0.1894	0.1057	240
SA-7	0.0550	0.0654	0.0570	0.1067	0.1293	0.1135	0.1469	0.1905	0.1149	240
SA-8	0.0639	0.0760	0.0666	0.1244	0.1379	0.1053	0.1209	0.1859	0.1028	300
SA-8	0.0647	0.0770	0.0669	0.1246	0.1345	0.1060	0.1197	0.1861	0.1058	300
SA-8	0.0573	0.0708	0.0621	0.1160	0.1359	0.1139	0.1415	0.1778	0.1046	300
SA-9	0.0560	0.0738	0.0634	0.1208	0.1399	0.1078	0.1229	0.1898	0.1091	360
SA-9	0.0531	0.0715	0.0624	0.1195	0.1396	0.1073	0.1251	0.1946	0.1096	360
SA-9	0.0548	0.0702	0.0619	0.1166	0.1389	0.1167	0.1428	0.1752	0.1034	360

Sample #	Benzene	2,2,4-trimethylpentane	Heptane	Toluene	m-Xylene	Nonane	Decane	1,2,3,5-tetramethylbenzene	Naphthalene	Weathering time (min)
SB-1	0.0990	0.0870	0.0733	0.1292	0.1275	0.0968	0.1038	0.1762	0.0944	1
SB-1	0.0855	0.0810	0.0706	0.1260	0.1302	0.0973	0.1119	0.1792	0.1023	1
SB-1	0.0877	0.0825	0.0710	0.1236	0.1295	0.1080	0.1298	0.1580	0.0926	1
SB-10	0.0419	0.0646	0.0572	0.1144	0.1411	0.1091	0.1296	0.2034	0.1197	480
SB-10	0.0470	0.0664	0.0589	0.1179	0.1440	0.1085	0.1277	0.1974	0.1134	480
SB-10	0.0450	0.0642	0.0568	0.1102	0.1359	0.1177	0.1485	0.1891	0.1121	480
SB-11	0.0325	0.0593	0.0524	0.1090	0.1441	0.1103	0.1343	0.2150	0.1228	600
SB-11	0.0370	0.0638	0.0558	0.1123	0.1453	0.1121	0.1283	0.2158	0.1132	600
SB-11	0.0392	0.0628	0.0557	0.1114	0.1411	0.1213	0.1503	0.1877	0.1098	600
SB-12	0.0310	0.0580	0.0515	0.1107	0.1476	0.1119	0.1344	0.2106	0.1239	720
SB-12	0.0335	0.0612	0.0530	0.1128	0.1469	0.1118	0.1328	0.2128	0.1186	720
SB-12	0.0264	0.0536	0.0474	0.1004	0.1427	0.1224	0.1567	0.2049	0.1219	720
SB-13	0.0111	0.0407	0.0365	0.0906	0.1512	0.1228	0.1510	0.2361	0.1377	1200
SB-13	0.0092	0.0346	0.0310	0.0781	0.1384	0.1165	0.1563	0.2581	0.1528	1200
SB-13	0.0117	0.0399	0.0363	0.0875	0.1463	0.1307	0.1705	0.2199	0.1322	1200
SB-14	0.0037	0.0267	0.0248	0.0722	0.1528	0.1287	0.1595	0.2567	0.1516	1680
SB-14	0.0031	0.0257	0.0236	0.0697	0.1488	0.1270	0.1625	0.2610	0.1542	1680
SB-14	0.0031	0.0233	0.0220	0.0636	0.1419	0.1334	0.1825	0.2502	0.1511	1680
SB-15	0	0.0153	0.0141	0.0523	0.1461	0.1314	0.1726	0.2810	0.1622	2160
SB-15	0	0.0150	0.0137	0.0519	0.1492	0.1319	0.1711	0.2802	0.1616	2160
SB-15	0	0.0138	0.0134	0.0477	0.1375	0.1362	0.1926	0.2655	0.1629	2160
SB-16	0	0.0043	0.0043	0.0238	0.1231	0.1247	0.1860	0.3146	0.1855	2880
SB-16	0	0.0054	0.0053	0.0284	0.1353	0.1326	0.1846	0.3027	0.1768	2880
SB-16	0	0.0051	0.0053	0.0280	0.1286	0.1372	0.2051	0.2850	0.1731	2880
SB-17	0	0.0015	0.0016	0.0126	0.1176	0.1310	0.1956	0.3237	0.1874	3600

Sample #	Benzene	2,2,4-trimethylpentane	Heptane	Toluene	m-Xylene	Nonane	Decane	1,2,3,5-tetramethylbenzene	Naphthalene	Weathering time (min)
SB-17	0	0.0012	0.0013	0.0115	0.1075	0.1202	0.1948	0.3299	0.1981	3600
SB-17	0	0.0014	0.0015	0.0132	0.1107	0.1300	0.2104	0.3074	0.1902	3600
SB-18	0	0	0	0	0.0952	0.1235	0.2025	0.3444	0.2027	4320
SB-18	0	0	0	0	0.0986	0.1196	0.2001	0.3420	0.2036	4320
SB-18	0	0	0	0.0054	0.0987	0.1325	0.2229	0.3151	0.1896	4320
SB-19	0	0	0	0	0.0741	0.1106	0.2017	0.3650	0.2149	5040
SB-19	0	0	0	0	0.0733	0.1100	0.2026	0.3627	0.2171	5040
SB-19	0	0	0	0	0.0789	0.1215	0.2279	0.3318	0.2023	5040
SB-2	0.0873	0.0803	0.0702	0.1262	0.1317	0.0972	0.1136	0.1763	0.1008	30
SB-2	0.0816	0.0805	0.0693	0.1243	0.1338	0.1001	0.1151	0.1775	0.1014	30
SB-2	0.0761	0.0747	0.0652	0.1137	0.1260	0.1085	0.1381	0.1743	0.1044	30
SB-20	0	0	0	0	0.0434	0.0893	0.2090	0.3863	0.2340	6360
SB-20	0	0	0	0	0.0444	0.0898	0.2083	0.3850	0.2330	6360
SB-20	0	0	0	0	0.0445	0.0955	0.2272	0.3644	0.2262	6360
SB-21	0	0	0	0	0.0107	0.0483	0.1973	0.4356	0.2632	7800
SB-21	0	0	0	0	0.0092	0.0477	0.1993	0.4379	0.2627	7800
SB-21	0	0	0	0	0.0130	0.0552	0.2167	0.4045	0.2631	7800
SB-3	0.0763	0.0800	0.0691	0.1223	0.1354	0.1000	0.1182	0.1808	0.1032	60
SB-3	0.0820	0.0815	0.0709	0.1243	0.1331	0.0998	0.1125	0.1810	0.1004	60
SB-3	0.0843	0.0809	0.0699	0.1236	0.1304	0.1085	0.1303	0.1607	0.0940	60
SB-4	0.0755	0.0796	0.0673	0.1229	0.1323	0.1023	0.1150	0.1851	0.1051	90
SB-4	0.0806	0.0790	0.0679	0.1237	0.1288	0.0986	0.1172	0.1825	0.1056	90
SB-4	0.0803	0.0772	0.0671	0.1198	0.1300	0.1073	0.1330	0.1668	0.0998	90
SB-5	0.0776	0.0809	0.0683	0.1240	0.1302	0.0987	0.1123	0.1888	0.1042	120
SB-5	0.0734	0.0794	0.0677	0.1228	0.1339	0.1016	0.1143	0.1865	0.1056	120

Sample #	Benzene	2,2,4-trimethylpentane	Heptane	Toluene	m-Xylene	Nonane	Decane	1,2,3,5-tetramethylbenzene	Naphthalene	Weathering time (min)
SB-5	0.0720	0.0774	0.0672	0.1202	0.1315	0.1111	0.1353	0.1685	0.0982	120
SB-6	0.0713	0.0762	0.0668	0.1239	0.1366	0.1011	0.1187	0.1843	0.1037	180
SB-6	0.0514	0.0656	0.0574	0.1080	0.1340	0.1051	0.1311	0.2056	0.1206	180
SB-6	0.0627	0.0702	0.0616	0.1122	0.1303	0.1106	0.1409	0.1819	0.1093	180
SB-7	0.0578	0.0733	0.0645	0.1192	0.1371	0.1058	0.1221	0.1942	0.1096	240
SB-7	0.0638	0.0737	0.0633	0.1188	0.1340	0.1023	0.1198	0.1940	0.1135	240
SB-7	0.0609	0.0706	0.0627	0.1141	0.1309	0.1128	0.1418	0.1800	0.1063	240
SB-8	0.0605	0.0733	0.0636	0.1207	0.1368	0.1035	0.1212	0.1935	0.1103	300
SB-8	0.0557	0.0694	0.0605	0.1142	0.1340	0.1052	0.1250	0.2025	0.1162	300
SB-8	0.0587	0.0702	0.0609	0.1138	0.1316	0.1106	0.1402	0.1833	0.1102	300
SB-9	0.0543	0.0722	0.0623	0.1187	0.1380	0.1071	0.1234	0.1974	0.1109	360
SB-9	0.0587	0.0739	0.0636	0.1225	0.1387	0.1053	0.1206	0.1937	0.1078	360
SB-9	0.0514	0.0641	0.0564	0.1076	0.1304	0.1098	0.1442	0.1947	0.1201	360

Appendix B

function f_tof_conv (INDIR, TRIM)

%This function will enter a directory specified by INDIR, collect a list of %all of the .csv
%files in the directory, and then convert them from %exported Chemstation format into
%a .prn file that is in the format that can be read into Leco's ChromaTOF. It will also trim
%off TRIM seconds of data.

%This version also includes checking for unicode files. If unicode csv files are found in
%the directory being processed, the files are converted to standard ascii encoding prior
%to conversion to the .prn files.

%I/O:

%INDIR - this is the directory where all of the .csv files are stored

%TRIM - the number of seconds of data to remove from the start of the run.

%This should be an even multiple of modulation periods for GCxGC data.

%There is no output passed from this function.

%The function does generate a series of files [filename].prn which are formatted to be
%imported into Leco ChromaTOF 4.xx. The files are placed in the same directory where
%the original data files were found.

%Warnings and limitations:

%Files in the input directory must all be formatted as two columns separated by a
%comma. Column 1 is the time associated with the data point, and Column 2 is the
%signal intensity at that time.

%This function (c) James Harynuk, March - Sept 2010 Version 1.2


```

% Check to see if INDIR ends in a \
if INDIR(end) ~= '\'
    INDIR = strcat(INDIR,'\');
end %if INDIR

FILES = dir(strcat(INDIR,'*.csv'));
% check for files that are unicode and rewrite them as ascii
for i = 1:length(FILES)
    INFILE = strcat(INDIR,FILES(i).name);
    if isunicode(INFILE)
        disp (strcat('Converting file ', INFILE,' to ascii'));
        unicode2ascii(INFILE);
    end %if isunicode
end %for loop to convert files

for i = 1:length(FILES)
    INFILE = strcat(INDIR,FILES(i).name);
    OUTFILE = strcat(INFILE(1:end-3), 'prn');
    disp (strcat('Converting file ', FILES(i).name,' to .prn format...'));

% Read in the data and pull out the time (column 1) and signal (column 2). Turn signal
%(S) into a row vector and chop off the decimal places after multiplying by 1000 to gain
%enough precision

TEMP = csvread(INFILE);
t = TEMP(:,1);
S = round(TEMP(:,2)*1000)';
clear TEMP;

% Figure out the data rate
period = diff(t); % Vector of periods in minutes
rate = round(1 / (period(1) * 60)); %Data rate in Hz

```

```

% Trim off initial portion of data or add some data to it

if TRIM >= 0 % Positive number means were are getting rid of data
    start = rate * TRIM + 1;
    S = S(start:end);

else % Negative number means we will add zeros to the beginning

    temp = S;
    zerosadd = rate * abs(TRIM);
    totalpoints = zerosadd + size(temp,2);
    S(1:zerosadd) = 0;
    S((zerosadd+1):totalpoints) = temp;

end

% Open the file to write data into
FID = fopen(OUTFILE,'w+');

% Write header information into the file
fprintf(FID, 'mass-spec-ascii\n1\n4\n%u\n%u\n', length(S), rate);
% Write Signal data into file
fprintf(FID,'%u ', S);
fclose(FID);

end %for FILES loop

disp ('Done converting files. ');
end %function

```

Appendix C

Appendix C

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2C-1_89	0.0000	0.0897	1.6001	0.9938	0.5693	0.4931	11.6645	0.5763	12.6491	7.7441	6.2795	1.4151	1.0692	2.2860
3C-13_87	0.0000	0.5707	5.8769	3.4600	2.0587	1.8939	1.4408	0.0215	4.3545	6.8238	5.8867	3.0081	2.4044	4.7743
3C-3_89	0.0000	0.1298	1.7496	1.0442	0.6023	0.5249	12.4170	0.6793	13.8187	8.6234	8.1008	1.5052	0.9818	2.4085
2C-10_87	0.0000	0.2524	6.8132	4.3892	2.6372	2.3759	6.0917	0.4250	7.4625	6.7678	8.4819	2.6751	1.9508	3.9050
3C-14_89	0.0000	0.3802	5.4616	3.3908	1.9971	1.7783	0.9083	0.0000	4.8178	8.4411	4.6170	2.0733	1.7237	5.4623
1A-7_87	0.0528	0.1551	7.1816	3.3091	0.5060	0.3886	9.4874	0.3728	3.8448	3.3687	0.7862	1.1070	0.3705	0.6702
3B-13_89	0.0000	0.3197	4.5716	2.8682	1.6997	1.4849	1.9695	0.0141	6.8896	9.4759	6.0305	2.1307	1.6571	4.9056
4C-13_87	0.0605	0.0672	3.5008	1.8460	0.4658	0.3255	2.3710	0.0524	9.3628	7.3299	9.1413	3.6429	2.9353	4.9557
3A-15_89	0.0000	0.5391	6.8050	4.4442	2.6572	2.3576	0.1004	0.0000	1.2224	4.8268	1.9015	1.6017	1.6381	5.8670
4B-6_87	0.0248	0.0351	1.8403	0.9505	0.2401	0.1575	9.9209	0.8145	18.7687	6.7349	11.3118	2.8032	1.9941	3.0650
2C-18_87	0.0000	1.8207	27.0378	22.0098	14.9928	15.0195	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3632
4A-4_87	0.0261	0.0314	1.7201	0.8978	0.2267	0.1576	10.4422	0.9081	9.6865	6.4230	10.8896	2.6776	1.8899	2.8932
2C-18_87	0.0000	1.8413	23.2070	18.8042	12.6385	13.7221	0.0054	0.0000	0.0047	0.0000	0.0000	0.0000	0.0000	0.3535

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2A-19_87	0.0000	2.4835	27.8368	27.1614	19.8519	23.0134	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0209
2A-16_87	0.0000	0.8570	15.0171	10.0029	6.2769	5.4735	0.0000	0.0000	0.0182	0.4747	0.1437	0.5907	1.1046	3.8489
2B-3_89	0.0000	0.1003	1.7856	1.1047	0.6343	0.5249	12.0647	0.5824	13.7316	8.6037	6.7905	1.4561	0.9688	2.4182
4A-17_87	0.2356	0.3196	11.4126	6.6127	1.7766	1.2985	0.0132	0.0000	0.0071	0.1192	0.0208	0.3312	0.9309	3.9470
2B-10_87	0.0000	0.3012	5.0211	3.0073	1.7915	1.4444	6.0654	0.2761	8.6473	7.6518	8.1606	2.8713	2.0775	3.7318
3A-5_87	0.0000	0.2625	2.9041	1.6806	1.0077	0.8929	12.2393	0.8618	10.4336	7.0679	8.3752	2.5171	1.6317	2.9912
1A-7_89	0.0509	0.1751	7.1275	3.4197	0.5627	0.4606	7.8652	0.4582	2.7496	2.3386	7.5130	0.7860	0.3041	0.5276
1B-10_87	0.0509	0.1786	10.3757	4.9359	0.7754	0.5563	7.0403	0.2596	3.3885	3.6070	0.8001	1.2023	0.4624	0.8534
2B-17_89	0.0000	1.1707	12.5068	8.9661	5.6229	5.4662	0.0000	0.0000	0.0000	0.0028	0.0000	0.0390	0.1241	1.8545
3B-10_87	0.0000	0.3497	3.6973	2.2203	1.2471	1.2028	7.9421	0.4129	9.7733	7.9425	8.6581	2.8890	2.0022	3.6273
1A-12_87	0.0644	0.2336	12.3656	5.9021	0.9385	0.7366	3.6703	0.1090	2.4594	3.3795	0.7511	1.2596	0.5340	0.8403
1B-19_87	0.2745	1.2239	41.0832	24.2419	4.3130	3.6555	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0938
3C-11_87	0.0000	0.3779	3.9748	2.3308	1.3433	1.3905	6.6751	0.3034	8.8400	7.7742	8.1695	2.8997	2.0604	3.7414
3A-6_87	0.0000	0.2872	3.0723	1.7737	1.0430	0.9189	12.1532	0.8270	10.6823	7.4568	8.7079	2.5789	1.7124	3.1049
1A-1_89	0.0214	0.1076	4.8920	2.3389	0.3442	0.2809	8.0331	0.5192	2.1914	1.6652	5.9053	0.5116	0.1906	0.3637
1A-4_87	0.0625	0.1399	4.3340	1.9172	0.3021	0.2161	11.5050	0.4323	4.0976	3.1745	0.6801	0.9935	0.4099	0.5915
1A-15_87	0.1544	0.4232	16.8275	8.1943	1.3456	1.0506	0.0200	0.0000	0.0654	0.7501	0.1142	0.5260	0.3677	0.8448
1C-4_87	0.0417	0.1265	5.7621	2.6707	0.4059	0.3145	9.1926	0.3698	3.3820	2.8843	0.6631	0.9307	0.3789	0.5743
3C-9_87	0.0000	0.3185	3.3533	1.9711	1.1746	1.0313	9.3490	0.5490	10.0455	7.5994	8.4813	2.7154	1.8549	3.3558

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2B-2_89	0.0000	0.0969	1.6851	1.0335	0.5979	0.5141	12.1566	0.5818	13.6612	8.3762	6.5419	1.4154	0.9161	2.3352
1B-19_87	0.3135	1.2700	35.0725	20.4789	3.5584	3.0717	0.0055	0.0000	0.0096	0.0000	0.0000	0.0000	0.0000	0.1112
2B-10_87	0.0000	0.2756	6.5272	4.1220	2.5613	2.1278	5.5655	0.3270	7.5004	7.1513	8.2447	2.7897	2.0320	3.8754
4A-14_87	0.0867	0.0918	4.6348	2.4823	0.6408	0.4453	0.4759	0.0000	3.4935	5.5670	5.4492	3.3549	3.0770	5.7737
3A-6_87	0.0000	0.2808	3.0562	1.8085	1.0105	0.9293	12.1765	0.8253	10.8468	7.4601	8.6828	2.6592	1.7404	3.1126
4C-3_87	0.0241	0.0283	1.6306	0.8397	0.2100	0.1388	10.3828	0.9171	9.5296	6.1645	10.5572	2.5544	1.8100	2.7675
4B-1_87	0.0158	0.0264	1.4843	0.7618	0.1951	0.1254	10.2125	0.9387	8.8766	5.6122	9.7721	2.3169	1.6380	2.4282
4C-5_87	0.0269	0.0307	1.7712	0.9172	0.2276	0.1535	10.1322	0.8698	20.3612	6.4509	10.8885	2.6879	1.8727	2.8651
3C-17_87	0.0000	1.6404	13.1739	8.7500	5.3412	5.6739	0.0107	0.0000	0.0057	0.0172	0.0042	0.0521	0.3007	2.0544
3B-17_89	0.0000	1.2321	13.2015	9.6707	6.0881	5.6299	0.0000	0.0000	0.0000	0.0124	0.0000	0.0299	0.1815	2.5705
1B-17_87	0.2061	0.6086	21.5119	10.8925	1.8220	1.4234	0.0051	0.0000	0.0050	0.0868	0.0059	0.1206	0.1589	0.5674
2C-8_89	0.0000	0.1185	1.6431	1.0075	0.5684	0.4847	9.9539	0.3625	12.9090	8.8083	6.3336	1.4731	0.9916	2.4363
2C-13_89	0.0000	0.2351	4.8744	3.0554	1.7694	1.5959	1.7708	0.0000	6.6184	9.0505	4.9487	2.0021	1.5389	4.7218
3C-3_87	0.0000	0.2602	2.7258	1.6123	0.9437	0.8525	12.8853	0.9274	10.3819	6.9833	8.2219	2.4294	1.6197	2.8910
2B-2_87	0.0000	0.1872	3.4356	2.0952	1.2876	1.1111	10.6457	0.8219	8.8011	5.9823	7.4054	2.1606	1.4691	2.7065
1A-11_89	0.0570	0.2232	11.2074	5.4756	0.8982	0.7086	4.3232	0.2712	2.1271	2.3454	8.1280	0.8242	0.3558	0.6663
3C-15_87	0.0000	0.8762	8.5083	5.2505	2.9634	3.1247	0.0399	0.0000	0.4051	2.4935	1.3781	1.6903	1.9158	4.7468
1B-1_87	0.0279	0.1368	6.9224	3.3662	0.5204	0.4135	7.6858	0.3061	2.6794	2.3519	0.5478	0.7443	0.2627	0.5037
1A-1_87	0.0426	0.1009	3.2654	1.4607	0.2269	0.1625	10.1241	0.3991	3.3424	2.4783	0.5426	0.7658	0.2940	0.4445

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2A-13_89	0.0000	0.2910	4.4413	2.8077	1.5977	1.3690	1.5364	0.0050	6.1497	9.6084	4.8217	2.2090	1.7451	5.2751
3B-1_87	0.0000	0.2004	2.1918	1.2975	0.7136	0.6736	12.1107	0.9111	9.2283	5.8568	6.9470	2.0582	1.3405	2.1997
1B-17_89	0.1932	0.8973	39.3993	22.5888	4.0719	3.4914	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1811
1A-6_89	0.0527	0.1630	6.4605	3.0715	0.5145	0.3911	7.9224	0.4581	2.7681	2.2809	7.3161	0.7884	0.3224	0.5253
3B-3_89	0.0000	0.1277	1.6493	0.9727	0.5610	0.4932	12.1317	0.6310	13.3879	8.3717	7.5159	1.4623	0.9526	2.3471
1C-14_89	0.1137	0.3708	15.8484	7.8664	1.3189	1.0629	0.0770	0.0000	0.1835	1.0079	2.9267	0.5293	0.3159	0.7147
3A-19_87	0.0000	2.5912	14.5306	11.5664	7.5068	8.1908	0.0148	0.0000	0.0065	0.0000	0.0000	0.0000	0.0000	0.2476
3C-5_89	0.0000	0.1349	1.8112	1.0780	0.6232	0.5163	12.3272	0.6335	14.0152	8.9149	8.2129	1.5524	1.0218	2.5420
1C-8_89	0.0603	0.1968	8.0098	3.8213	0.6366	0.4989	7.3128	0.4291	2.8605	2.5442	8.1960	0.8630	0.3605	0.6060
3B-11_87	0.0000	0.4105	4.2404	2.5047	1.4755	1.3501	6.4123	0.2837	9.2778	8.3548	8.7364	3.1340	2.2128	4.0132
2A-4_87	0.0000	0.1836	3.9177	2.5246	1.5008	1.3455	10.5180	0.8371	8.6387	6.2296	7.7954	2.3223	1.5077	2.8492
3C-10_89	0.0000	0.1726	2.6609	1.6221	0.9582	0.8709	8.5293	0.3222	12.2021	9.6468	8.4393	1.7808	1.2416	3.1986
4C-11_87	0.0293	0.0422	2.3919	1.2479	0.3099	0.2056	6.5552	0.3597	8.8840	7.4661	11.2843	3.2903	2.4342	3.8621
1C-3_89	0.0381	0.1369	5.4905	2.6146	0.4226	0.3325	7.9460	0.4694	2.4928	1.9724	6.4970	0.6515	0.2656	0.4258
3B-5_89	0.0000	0.1293	1.7375	1.0354	0.6050	0.5118	11.1920	0.5651	12.9609	8.2789	7.6780	1.4653	0.9443	2.3924
2C-12_89	0.0000	0.1880	3.2023	2.0362	1.1884	0.9932	6.1565	0.1381	12.2792	10.5824	7.2081	1.9882	1.4517	3.8896
3B-6_87	0.0000	0.2871	3.0432	1.7663	1.0425	0.9432	11.4570	0.7741	10.2614	7.2049	8.4328	2.5552	1.6845	3.0039
3A-3_89	0.0000	0.1301	1.6996	1.0229	0.5854	0.4797	12.4762	0.6621	13.7936	8.6407	7.9761	1.5046	0.9586	2.4334
3B-9_87	0.0000	0.3476	3.7305	2.1834	1.2761	1.1428	10.0828	0.6002	10.8125	8.2824	9.3968	2.9618	1.9787	3.6524

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
3A-15_87	0.0000	0.8136	8.0594	4.8240	2.8824	2.9294	0.0719	0.0000	0.6883	3.1849	1.8927	1.9357	2.0362	5.0735
4A-6_87	0.0286	0.0320	1.8531	0.9702	0.2416	0.1655	9.9807	0.8121	9.7278	6.7200	11.1561	2.8172	2.0142	3.1114
1A-15_87	0.1520	0.4237	15.7251	7.6414	1.2487	0.9589	0.0155	0.0000	0.0659	0.7740	0.1105	0.5304	0.3661	0.8442
2B-13_89	0.0000	0.3111	5.2447	3.3068	1.8910	1.6689	1.2966	0.0000	5.6884	9.1268	4.5052	2.0974	1.7128	5.4300
1A-3_89	0.0401	0.1529	6.2716	3.0115	0.4709	0.3797	7.7164	0.4330	2.4082	2.0128	6.2650	0.6496	0.2641	0.4654
3C-10_87	0.0000	0.3361	3.5640	2.1175	1.2026	1.1009	7.9374	0.4301	9.5578	7.7167	8.3814	2.8044	1.9360	3.5247
2A-13_87	0.0000	0.4152	9.3156	5.9560	3.7014	3.2140	1.3014	0.0242	3.9445	6.0928	5.8032	2.7639	2.3278	4.9034
3C-2_89	0.0000	0.1130	1.5964	0.9548	0.5446	0.4897	11.2505	0.6197	11.7440	7.7522	7.0469	1.3375	0.8496	2.1571
4C-17_87	0.2535	0.3316	11.8584	6.9605	1.9306	1.3700	0.0163	0.0000	0.0067	0.0763	0.0116	0.2575	0.8103	3.7473
2A-19_87	0.0000	2.4837	25.0274	24.6485	17.9156	20.5468	0.0000	0.0000	0.0056	0.0000	0.0000	0.0000	0.0000	0.0344
1C-19_87	0.3770	3.1630	44.9622	37.1609	7.3107	7.5531	0.0000	0.0000	0.0055	0.0000	0.0000	0.0000	0.0000	0.0000
4C-7_87	0.0236	0.0346	1.9469	1.0208	0.2517	0.1628	9.7881	0.7608	22.0711	7.0125	11.6067	2.9616	2.1097	3.2682
1C-4_87	0.0473	0.1290	5.1526	2.3628	0.3414	0.2729	9.7744	0.3834	3.6080	2.9762	0.6677	0.9581	0.3804	0.5713
3A-14_89	0.0000	0.4224	5.7763	3.6368	2.1553	1.9202	0.5441	0.0000	3.4228	7.4996	3.8199	1.9989	1.7403	5.6174
2C-4_87	0.0000	0.1981	4.1269	2.6648	1.6354	1.4302	10.3207	0.8080	8.7860	6.4846	8.0541	2.3344	1.6087	2.8550
4C-4_87	0.0264	0.0265	1.7274	0.8867	0.2243	0.1434	10.3954	0.8744	21.2221	6.4178	10.8530	2.6695	1.8913	2.8850
1C-8_87	0.0431	0.1573	9.2563	4.4314	0.6422	0.5212	8.6099	0.3825	3.4828	3.3182	0.8152	1.1134	0.4198	0.7203
1B-12_89	0.0827	0.2612	10.6077	5.1118	0.8498	0.6756	2.5797	0.1239	1.7493	2.4504	7.3266	0.9266	0.4182	0.7334
3A-13_89	0.0000	0.3215	4.7687	2.9700	1.7808	1.5606	2.0474	0.0162	6.8100	9.4960	6.2081	2.1365	1.6283	4.8727

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2B-3_87	0.0000	0.2029	3.6590	2.2726	1.3844	1.1408	10.5448	0.7760	9.0035	6.4639	7.9177	2.3118	1.5712	2.7501
3B-7_89	0.0000	0.1545	2.2921	1.3806	0.8081	0.6927	11.1628	0.5294	13.8958	9.6307	8.8086	1.7285	1.1404	2.8930
1B-16_87	0.1530	0.4681	19.1594	9.5249	1.5394	1.2226	0.0000	0.0000	0.0088	0.3843	0.0500	0.3098	0.2692	0.7714
3A-16_89	0.0000	0.7313	10.4848	6.9278	4.1997	3.8526	0.0000	0.0000	0.1093	1.1247	0.2027	0.6799	1.0200	5.3860
3A-14_89	0.0000	0.4192	6.1971	3.8951	2.3289	2.0905	0.5199	0.0000	3.3783	7.3821	3.7994	1.9837	1.6980	5.6785
3A-15_87	0.0000	0.8114	7.9092	4.7822	2.8502	2.7889	0.0703	0.0000	0.6922	3.1995	1.8718	1.9463	2.0473	5.1162
4B-12_87	0.0424	0.0479	2.5985	1.3641	0.3416	0.2288	5.6042	0.2678	15.1441	7.4711	11.0098	3.3848	2.5356	4.0151
1B-8_87	0.0485	0.1580	8.3490	3.9580	0.5872	0.4594	9.0949	0.3538	3.7015	3.4437	0.7955	1.1181	0.3976	0.7232
3C-5_87	0.0000	0.2732	2.9203	1.6868	0.9876	0.8793	12.5738	0.8731	10.7789	7.2798	8.5751	2.5468	1.6844	3.0144
2C-4_87	0.0000	0.1901	4.2531	2.7144	1.6799	1.4984	10.4840	0.8317	8.8272	6.4550	8.0650	2.3591	1.6229	2.9908
3A-3_89	0.0000	0.1290	1.7879	1.0697	0.6175	0.5392	12.1843	0.6537	13.3692	8.5733	8.0304	1.4681	0.9417	2.4187
3A-6_89	0.0000	0.1465	2.1468	1.2947	0.7458	0.6753	11.0502	0.5395	13.3875	9.2276	8.3992	1.6250	1.0564	2.7372
2B-6_87	0.0000	0.1958	4.7240	3.1102	1.8296	1.6315	10.4708	0.9003	8.9586	6.5713	8.7681	2.4540	1.6423	3.0316
3A-5_89	0.0000	0.1381	1.8703	1.1333	0.6430	0.5516	11.4227	0.5899	13.4016	8.6459	7.9122	1.5246	1.0170	2.5295
3B-1_87	0.0000	0.1987	2.1743	1.2852	0.7278	0.6997	12.3228	0.9217	9.3358	5.8936	7.0234	2.0722	1.3398	2.4074
1B-12_87	0.0769	0.2382	9.8035	4.5842	0.7360	0.5427	4.8505	0.1242	3.0408	3.7730	0.7868	1.3536	0.5975	0.9308
1A-10_87	0.0444	0.1998	10.9397	5.2154	0.8438	0.6386	5.8067	0.2012	3.0531	3.4782	0.7715	1.2095	0.4423	0.8712
2C-1_87	0.0000	0.1443	2.9602	1.8815	1.0671	0.9178	10.5945	0.9051	7.7003	5.1954	6.6738	1.8909	1.2184	2.1353
2A-9_87	0.0000	0.2666	4.5743	2.7897	1.6562	1.3652	6.7539	0.4386	8.8895	7.4022	8.3955	2.7271	1.8996	3.4206

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
3B-16_87	0.0000	1.2631	11.3844	7.1469	4.2846	4.4630	0.0119	0.0000	0.0056	0.2737	0.0559	0.3881	0.8623	3.6147
1C-15_89	0.1321	0.4441	17.6653	8.8125	1.5215	1.1949	0.0000	0.0000	0.0318	0.4500	1.2558	0.3038	0.2369	0.6464
1B-3_89	0.0411	0.1356	5.2086	2.4527	0.4055	0.3097	8.2662	0.4790	2.5748	1.9919	6.6370	0.6660	0.2673	0.4461
2B-1_87	0.0000	0.1325	2.8813	1.7426	1.0620	0.9426	9.9443	0.7992	7.5200	5.0979	6.2907	1.7926	1.2278	2.1533
3A-2_89	0.0000	0.1141	1.5441	0.9173	0.5263	0.4549	11.4589	0.6211	12.6653	7.7955	7.2567	1.3629	0.8739	2.2041
1C-17_87	0.2344	0.8157	30.0825	16.1427	2.7848	2.2625	0.0000	0.0000	0.0000	0.0000	0.0000	0.0229	0.0221	0.2941
1A-16_89	0.1506	0.5116	20.5501	10.4722	1.8326	1.4742	0.0000	0.0000	0.0073	0.2911	0.7304	0.2242	0.1998	0.6131
4B-2_87	0.0239	0.0277	1.6270	0.8391	0.2101	0.1412	10.1142	0.9244	19.7198	5.9762	10.3543	2.4870	1.7619	2.6825
1C-14_87	0.1343	0.3817	14.7645	7.0635	1.1434	0.8761	0.0910	0.0000	0.2777	1.4659	0.2418	0.8439	0.4607	0.9704
1C-12_89	0.0735	0.2585	11.8846	5.8004	0.9866	0.7739	2.9572	0.1500	1.8244	2.3837	7.7094	0.8928	0.3884	0.7105
4C-12_87	0.0372	0.0445	2.4745	1.2888	0.3282	0.2134	5.4618	0.2565	15.1123	7.3141	10.6442	3.3063	2.4725	3.9054
2C-11_89	0.0000	0.1503	2.6191	1.6663	0.9657	0.8103	6.2794	0.1460	11.2133	9.1174	6.4100	1.7098	1.2088	3.1996
1B-9_89	0.0622	0.2085	8.5810	4.1206	0.6849	0.5410	6.6038	0.3620	2.6671	2.4803	8.1708	0.8788	0.3629	0.6120
2C-9_89	0.0000	0.1270	1.8657	1.1406	0.6545	0.5777	9.9271	0.3398	13.6070	9.4241	6.7506	1.6141	1.0964	2.7349
3B-15_89	0.0000	0.5450	8.1225	5.2862	3.1580	2.8725	0.0712	0.0000	0.9476	4.2491	1.5545	1.5095	1.5537	6.1024
1B-3_87	0.0551	0.1267	3.9283	1.7437	0.2802	0.1979	11.0715	0.4187	3.7760	2.9089	0.6223	0.9168	0.3608	0.5319
4A-15_87	0.1278	0.1361	6.2085	3.3622	0.9046	0.6326	0.0826	0.0000	1.0784	3.7789	2.9350	2.7905	2.9940	6.3291
2A-6_89	0.0000	0.1198	2.1252	1.3165	0.7608	0.6386	11.7438	0.5116	14.3993	9.5537	7.4870	1.6546	1.0955	2.7921
1B-15_87	0.1347	0.3843	15.4647	7.5086	1.2192	0.9333	0.0548	0.0000	0.1823	1.2313	0.1898	0.7274	0.4554	0.9368

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
1C-8_89	0.0447	0.1916	8.2081	3.9618	0.6785	0.5140	7.5445	0.4456	2.7285	2.4503	8.1898	0.8284	0.3078	0.5808
2C-19_87	0.0000	2.1443	25.8958	23.1677	16.2364	17.9961	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1089
1A-15_89	0.1113	0.3947	17.8733	8.9506	1.5196	1.2326	0.0441	0.0000	0.1237	0.8344	2.3012	0.5004	0.2989	0.6975
4A-8_87	0.0311	0.0384	2.0288	1.0566	0.2680	0.1850	8.8460	0.6593	19.6307	6.9316	11.2888	2.9596	2.1232	3.3091
2C-4_87	0.0000	0.1918	3.9486	2.5170	1.5450	1.2798	10.3481	0.7752	8.8364	6.3552	7.8699	2.3149	1.6075	2.8320
3A-5_87	0.0000	0.2675	2.8926	1.6849	1.0009	0.8975	12.1602	0.8620	10.5393	7.0321	8.3465	2.4690	1.6257	2.9808
1A-13_87	0.1276	0.3163	11.7531	5.5591	0.8825	0.6685	0.5453	0.0042	0.8942	2.4547	0.4276	1.0849	0.5564	0.9787
1A-3_89	0.0488	0.1589	5.9147	2.8022	0.4543	0.3571	7.8969	0.4224	2.5260	2.0482	6.4655	0.6736	0.2951	0.4568
4C-14_87	0.0829	0.0930	4.6138	2.4538	0.6520	0.4526	0.7441	0.0063	4.7269	6.1645	6.3947	3.4476	3.1476	5.7731
4B-8_87	0.0309	0.0362	2.0495	1.0668	0.2682	0.1828	9.0001	0.6768	20.6338	7.0476	11.5875	2.9844	2.1370	3.2493
1C-1_87	0.0474	0.1043	3.1961	1.4324	0.2097	0.1581	9.7737	0.3767	3.2281	2.4203	0.5196	0.7575	0.3014	0.4368
3B-11_87	0.0000	0.4113	4.2700	2.5584	1.4456	1.4473	6.4055	0.2808	9.2691	8.3812	8.7642	3.0978	2.1952	4.1414
3C-14_87	0.0000	0.6587	6.5585	3.8803	2.3375	2.3407	0.3865	0.0000	2.0356	4.9838	3.6998	2.4875	2.2391	4.9581
3B-15_89	0.0000	0.5421	7.9767	5.1467	3.0830	2.7798	0.0694	0.0000	0.9579	4.2832	1.5731	1.5240	1.5831	6.0796
2B-12_87	0.0000	0.3399	7.0132	4.4646	2.7365	2.2839	3.3134	0.1501	6.3575	7.1444	7.5341	2.9230	2.2464	4.3822
2A-14_87	0.0000	0.5295	10.4129	6.7228	4.1326	3.4409	0.3379	0.0000	1.7302	4.5671	3.6729	2.4443	2.2839	5.0677
1B-16_89	0.1872	0.6907	27.3473	14.5609	2.5077	2.1336	0.0000	0.0000	0.0000	0.0314	0.0766	0.0640	0.0524	0.3753
3C-15_87	0.0000	0.8827	8.5517	5.1566	3.0474	3.0273	0.0416	0.0000	0.4253	2.4884	1.3676	1.7164	1.9381	4.6490
1B-9_89	0.0707	0.2092	8.3235	3.9650	0.6769	0.5116	6.7047	0.3596	2.8100	2.5972	8.2486	0.9056	0.4028	0.6182

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2B-18_89	0.0000	1.8014	12.5483	11.1957	7.6575	8.0446	0.0067	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2183
2A-5_89	0.0000	0.1137	1.9024	1.1871	0.6748	0.5578	12.1624	0.5506	14.5104	9.1555	7.1825	1.5520	1.1024	2.6648
2A-2_89	0.0000	0.0952	1.6875	1.0400	0.6007	0.4944	12.0895	0.5972	12.7764	8.3128	6.6228	1.4056	0.9163	2.3006
2B-10_87	0.0000	0.2998	5.1198	3.1305	1.8757	1.5447	5.2970	0.2775	8.1761	7.5831	8.2608	2.8640	2.0470	3.7457
1C-2_89	0.0373	0.1356	5.4092	2.5731	0.4178	0.3226	8.1784	0.4972	2.5570	1.9961	6.5303	0.6332	0.2578	0.4348
4A-17_87	0.2413	0.3169	11.2945	6.4762	1.8099	1.2875	0.0060	0.0000	0.0066	0.1119	0.0195	0.3268	0.9208	3.9685
3A-8_89	0.0000	0.1429	2.2226	1.3522	0.7803	0.7078	8.6200	0.3772	11.7233	8.5005	7.4703	1.5623	1.0047	2.7025
1A-18_89	0.2053	0.7991	30.3395	16.5268	2.9515	2.4234	0.0000	0.0000	0.0000	0.0000	0.0000	0.0214	0.0318	0.2879
3B-9_89	0.0000	0.1704	2.5264	1.5153	0.8919	0.7999	10.1067	0.4165	13.8793	10.1118	8.9489	1.8431	1.2008	3.1663
2B-5_87	0.0000	0.1938	4.0641	2.5764	1.4854	1.2595	9.7798	0.7242	8.6523	6.3742	7.8912	2.3360	1.5448	2.8308
3C-16_89	0.0000	0.6750	7.6351	5.0194	2.9741	2.6298	0.0084	0.0000	0.3128	2.2308	0.5646	1.0323	1.3204	5.6369
1C-11_89	0.0776	0.2449	9.6573	4.6042	0.7964	0.6178	4.2635	0.2149	2.3775	2.6266	8.0745	0.9674	0.4430	0.6947
4B-3_87	0.0233	0.0298	1.6311	0.8357	0.2155	0.1434	10.5161	0.9193	20.1812	6.2665	10.5560	2.6064	1.8322	2.7402
3C-8_87	0.0000	0.3179	3.3258	1.9325	1.1349	1.0125	10.1370	0.6249	10.3664	7.5451	8.5926	2.7061	1.8200	3.2987
4B-14_87	0.2076	0.2857	10.5887	6.0351	1.6709	1.1815	0.0277	0.0000	0.0843	0.3312	0.2084	0.5240	1.1386	4.2868
3C-5_89	0.0000	0.1384	1.6501	0.9773	0.5610	0.4686	12.7606	0.6372	14.3161	8.9065	8.2250	1.5819	1.0187	2.4942
3A-12_87	0.0000	0.4059	4.2414	2.4670	1.4755	1.3781	5.0361	0.2307	8.5105	7.9940	8.2621	3.0171	2.1343	3.9982
2A-5_87	0.0000	0.1884	3.9390	2.4313	1.4349	1.2506	9.7876	0.7169	8.7983	6.2432	7.6426	2.2579	1.5765	2.8260
3B-2_89	0.0000	0.1171	1.6723	0.9984	0.5721	0.4982	12.1606	0.6844	13.3374	8.3786	7.8388	1.4419	0.9217	2.3109

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
3A-4_87	0.0000	0.2488	2.7152	1.5706	0.9254	0.8278	12.4216	0.8908	10.2132	6.7956	8.1218	2.4085	1.5544	2.8000
3C-18_89	0.0000	1.1932	13.1415	9.3407	5.8621	5.3524	0.0053	0.0000	0.0058	0.0123	0.0000	0.0300	0.1823	2.4336
3B-7_87	0.0000	0.3067	3.3078	1.9144	1.1178	1.0053	11.4995	0.7428	10.8780	7.8284	9.0964	2.7583	1.8434	3.2870
2B-17_89	0.0000	1.1375	13.7673	10.2771	6.4268	5.8683	0.0000	0.0000	0.0000	0.0000	0.0000	0.0038	0.0713	1.8642
2B-2_87	0.0000	0.1770	3.7342	2.3729	1.4909	1.2800	11.2303	0.9124	8.6300	5.9805	7.6466	2.1615	1.4553	2.5946
1A-19_89	0.2886	1.2569	39.0413	22.7047	4.1478	3.5417	0.0054	0.0000	0.0053	0.0000	0.0000	0.0000	0.0000	0.1007
2C-18_89	0.0000	1.9579	11.4512	10.7550	7.5502	8.0540	0.0063	0.0000	0.0059	0.0000	0.0000	0.0000	0.0000	0.1490
1B-18_89	0.3771	5.6897	46.8787	55.5994	12.7944	16.7301	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0337
3B-4_89	0.0000	0.1317	1.7416	1.0278	0.5862	0.5114	12.8058	0.6534	14.2793	8.9464	8.0140	1.5512	1.0162	2.4931
3B-18_87	0.0000	3.0084	13.8357	12.0338	8.2642	9.2765	0.0105	0.0000	0.0078	0.0000	0.0000	0.0000	0.0000	0.0610
2A-1_89	0.0000	0.0893	1.6722	1.0494	0.5773	0.5156	11.8482	0.6010	12.2611	7.9055	6.3497	1.3109	0.8699	2.1583
2B-8_87	0.0000	0.2412	5.8875	3.7133	2.2631	1.9085	7.4847	0.5364	8.2135	6.8571	8.4989	2.5660	1.7943	3.5444
2B-7_89	0.0000	0.1343	2.0743	1.2434	0.7076	0.6041	11.5727	0.4526	14.8081	9.8002	7.4158	1.6668	1.1330	2.8445
4A-7_87	0.0298	0.0360	1.9243	1.0072	0.2570	0.1689	9.4287	0.7302	9.7476	6.8712	11.2180	2.8878	2.0775	3.1744
3C-6_89	0.0000	0.1398	2.0819	1.2613	0.7391	0.6667	10.3987	0.5199	12.0086	8.6165	7.6786	1.5310	1.0046	2.6212
3A-18_89	0.0000	1.3275	12.6898	9.6666	6.1556	5.7191	0.0064	0.0000	0.0000	0.0021	0.0000	0.0072	0.0636	1.6803
1B-16_87	0.1557	0.4716	17.9865	8.8815	1.4616	1.1414	0.0062	0.0000	0.0151	0.3959	0.0541	0.3236	0.2556	0.7615
2C-13_87	0.0000	0.4060	8.6043	5.4295	3.3196	2.8203	1.1105	0.0187	3.5652	5.9153	5.4810	2.6828	2.2484	4.7184
3A-9_89	0.0000	0.1680	2.5936	1.5827	0.9293	0.8549	8.9847	0.3654	12.3499	9.5358	8.2969	1.7450	1.1633	3.0807

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
4B-5_87	0.0247	0.0312	1.7526	0.9094	0.2273	0.1513	10.1842	0.8740	21.0480	6.4070	10.8531	2.6790	1.9060	2.8406
2C-5_89	0.0000	0.1148	1.8470	1.1422	0.6592	0.5556	12.4442	0.5562	14.4536	9.1265	7.1406	1.5615	1.0376	2.5799
3B-6_89	0.0000	0.1388	2.0730	1.2457	0.7315	0.6507	11.2633	0.5600	13.3997	9.0458	8.0969	1.6030	1.0372	2.6687
2C-2_89	0.0000	0.0850	1.2934	0.7779	0.4215	0.3849	10.7727	0.5134	11.8671	7.1017	5.6060	1.1788	0.7835	1.9654
2B-10_89	0.0000	0.1544	2.3005	1.4423	0.8218	0.7282	8.1620	0.2348	12.9777	9.7579	6.8855	1.7738	1.2189	3.1517
1A-1_87	0.0499	0.1038	3.2837	1.4704	0.2210	0.1633	10.1325	0.3951	3.3293	2.4701	0.5401	0.7733	0.2998	0.4325
3A-7_87	0.0000	0.3040	3.2281	1.8842	1.1155	1.0165	11.4905	0.7454	10.7612	7.6111	8.7841	2.7034	1.7921	3.2456
1C-7_89	0.0521	0.1746	7.8919	3.8240	0.6476	0.5015	7.9561	0.4574	2.6456	2.3225	7.8060	0.8082	0.3237	0.5634
1A-8_89	0.0479	0.1811	8.2375	4.0070	0.6520	0.5047	7.3700	0.4689	2.6120	2.3639	8.1759	0.7852	0.2943	0.5677
4C-8_87	0.0282	0.0363	2.0673	1.0702	0.2634	0.1783	9.3509	0.6993	10.1951	7.2252	11.7928	3.0699	2.2001	3.4096
3A-8_87	0.0000	0.3309	3.5003	2.0381	1.1976	1.0869	11.2088	0.7082	11.2143	8.1093	9.3795	2.8808	1.8969	3.4471
1C-11_89	0.0777	0.2400	9.2649	4.4020	0.7401	0.5729	4.3260	0.2131	2.3066	2.6209	7.9384	0.9652	0.4358	0.6940
2C-12_89	0.0000	0.1904	3.2820	2.1052	1.2179	1.0434	6.1125	0.1256	11.5668	10.5246	7.1728	1.9769	1.4381	3.9171
2B-3_89	0.0000	0.1070	1.7399	1.0450	0.5926	0.5185	12.4478	0.5896	14.1668	8.7259	6.8653	1.4316	0.9648	2.4562
3B-13_89	0.0000	0.3144	4.7783	2.9548	1.7621	1.5466	1.9492	0.0134	6.8499	9.4432	6.0587	2.1438	1.6824	4.9499
1B-4_87	0.0639	0.1377	4.2011	1.8697	0.3011	0.2107	11.2804	0.4211	3.9570	3.0844	0.6572	0.9598	0.3863	0.5679
1B-15_87	0.1249	0.3783	16.4115	8.0128	1.2925	1.0240	0.0580	0.0000	0.1668	1.2053	0.1921	0.7000	0.4243	0.9278
3A-7_89	0.0000	0.1567	2.1887	1.3354	0.7825	0.6844	10.9915	0.4894	15.6776	9.5016	8.5870	1.6946	1.1464	2.9039
1C-19_87	0.3792	3.1558	45.1672	37.5833	7.4199	7.6716	0.0000	0.0000	0.0058	0.0000	0.0000	0.0000	0.0000	0.0000

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
1B-3_87	0.0586	0.1271	3.9531	1.7551	0.2828	0.1918	11.1194	0.4238	3.8386	2.9355	0.6283	0.9150	0.3587	0.5300
2B-3_87	0.0000	0.1978	3.6536	2.2545	1.3260	1.1641	9.4712	0.8266	9.5659	6.5212	7.7591	2.3234	1.5774	2.8272
3A-6_87	0.0000	0.2884	3.0580	1.7752	1.0479	0.9836	12.1677	0.8291	10.7524	7.4487	8.6810	2.6489	1.7154	3.1056
2A-8_87	0.0000	0.2441	4.7422	2.9295	1.7807	1.4723	8.6245	0.5759	9.0488	7.2285	8.3867	2.6307	1.8378	3.5251
1B-9_89	0.0655	0.2087	8.6999	4.1952	0.7074	0.5363	6.7117	0.3583	2.6712	2.5623	8.2672	0.9050	0.3771	0.6318
1A-13_87	0.1348	0.3254	10.9291	5.1471	0.7847	0.6347	0.6109	0.0051	0.9379	2.5213	0.4299	1.1039	0.5474	0.9839
3B-6_87	0.0000	0.2837	3.0214	1.7563	1.0333	0.9290	11.5421	0.7682	10.3414	7.2255	8.3526	2.5359	1.6799	3.0169
3C-2_87	0.0000	0.2363	2.5439	1.4822	0.8706	0.7905	12.2268	0.8878	9.8457	6.3652	7.5876	2.2314	1.4927	2.6167
2A-8_89	0.0000	0.1291	1.8269	1.0885	0.6093	0.5213	10.7397	0.3859	14.1789	9.7439	6.8807	1.6181	1.0755	2.6882
1A-8_89	0.0517	0.1824	7.5412	3.6332	0.5896	0.4648	7.5507	0.4314	2.7591	2.4452	7.9992	0.8367	0.3393	0.5673
2B-12_89	0.0000	0.1859	3.3954	2.1690	1.2588	1.0810	4.5864	0.0838	10.4067	9.5901	6.4324	1.8479	1.3993	3.8382
4C-12_87	0.0321	0.0457	2.4807	1.2940	0.3243	0.2155	5.5160	0.2619	14.8453	7.3730	10.6456	3.3132	2.4810	3.9837
3C-1_89	0.0000	0.1187	1.4653	0.8561	0.4759	0.4245	12.2239	0.6579	12.8989	7.8831	7.3371	1.3684	0.8899	2.1729
3C-3_89	0.0000	0.1310	1.6167	0.9433	0.5385	0.4653	12.9139	0.6708	8.3098	8.8875	8.1041	1.5119	0.9944	2.4236
2B-1_87	0.0000	0.1325	2.7232	1.7570	1.0293	0.9360	9.9677	0.8042	7.4522	5.0995	6.3237	1.8448	1.2067	2.1151
4B-3_87	0.0224	0.0282	1.6315	0.8471	0.2143	0.1410	10.3931	0.9177	20.9762	6.2072	10.5058	2.5605	1.7985	2.7590
2C-14_89	0.0000	0.3685	5.3717	3.4530	1.9497	1.6676	0.4292	0.0000	3.0970	7.3187	2.9695	1.9688	1.7826	5.7211
1A-10_89	0.0685	0.2134	8.1626	3.8757	0.6432	0.5035	6.0344	0.3097	2.6166	2.5743	7.9465	0.8989	0.3777	0.6439
1C-3_87	0.0577	0.1260	3.9336	1.7439	0.2790	0.1968	11.0710	0.4193	3.7938	2.9096	0.6264	0.9108	0.3673	0.5360

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2B-15_89	0.0000	0.5193	7.5890	5.0155	2.8933	2.5509	0.0184	0.0000	0.4626	2.7341	0.6462	1.1339	1.3453	5.8275
3C-13_89	0.0000	0.3111	4.2489	2.6093	1.5348	1.3446	2.7645	0.0295	8.0253	10.1428	6.7745	2.1842	1.6323	4.7614
1C-1_87	0.0483	0.0988	3.1930	1.4213	0.2231	0.1565	9.8340	0.3815	3.2376	2.4380	0.5210	0.7634	0.3049	0.4423
2A-16_89	0.0000	0.6754	9.8672	6.5434	3.8441	3.3118	0.0000	0.0000	0.0137	0.6029	0.0554	0.4184	0.8024	5.0925
2B-11_89	0.0000	0.1736	2.6638	1.6765	0.9572	0.7901	6.6415	0.1473	12.3360	10.2746	6.6615	1.8933	1.3472	3.5379
1A-11_89	0.0762	0.2387	8.7617	4.1383	0.6964	0.5502	4.6134	0.2156	2.4091	2.6404	7.9105	0.9636	0.4177	0.6855
2A-11_87	0.0000	0.3050	5.6401	3.5258	2.1164	1.7480	5.1731	0.2376	7.5780	7.1769	7.7811	2.8270	2.0751	4.0005
1C-18_89	0.3265	1.8831	50.3300	33.2456	6.2790	5.7891	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0133
1B-8_89	0.0560	0.1959	7.7564	3.7316	0.6104	0.4792	7.1218	0.3955	2.7658	2.4505	7.9835	0.8332	0.3465	0.5838
2A-7_87	0.0000	0.2348	4.4623	2.7616	1.6495	1.3625	8.6067	0.5532	8.7956	6.8388	8.1119	2.5061	1.7570	3.3528
1A-18_87	0.3742	1.1366	22.1071	11.9407	2.0325	1.6010	0.0107	0.0000	0.0074	0.0000	0.0000	0.0042	0.0048	0.1359
1A-16_87	0.1589	0.5323	23.0324	11.7011	1.9539	1.5420	0.0000	0.0000	0.0000	0.1499	0.0194	0.1736	0.1693	0.5955
1A-13_87	0.1076	0.3174	12.1078	5.7326	0.9115	0.7133	0.5500	0.0044	0.8877	2.4807	0.4405	1.0918	0.5586	0.9834
4B-14_87	0.2202	0.2847	10.6974	6.0874	1.6929	1.1966	0.0253	0.0000	0.0947	0.3326	0.2051	0.5244	1.1563	4.2847
2C-11_87	0.0000	0.2922	6.2251	3.9144	2.4301	2.0204	5.4031	0.2881	7.6279	7.3216	8.1455	2.8454	2.0673	3.9249
1A-14_87	0.1300	0.3620	13.9585	6.6734	1.0883	0.8299	0.1127	0.0000	0.3136	1.5495	0.2539	0.8452	0.4738	0.9482
2B-5_89	0.0000	0.1166	1.8420	1.1358	0.6452	0.5376	11.5730	0.5189	13.9496	8.7795	6.8354	1.6655	1.3849	2.8886
3A-9_87	0.0000	0.3369	3.5453	2.0759	1.2168	1.0990	10.2006	0.6064	6.1632	8.0954	0.0119	2.8668	1.9136	3.5210
3B-8_89	0.0000	0.1593	2.3005	1.3913	0.8025	0.7160	10.3026	0.4508	13.6916	9.6320	8.4290	1.7455	1.1549	2.9343

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2A-6_89	0.0000	0.1213	2.0856	1.3058	0.7491	0.6144	11.7463	0.5006	14.5635	9.6157	7.4020	1.6667	1.1029	2.8128
4A-8_87	0.0312	0.0383	2.0228	1.0581	0.2654	0.1826	8.8129	0.6592	19.1674	6.8919	11.2990	2.9398	2.1015	3.2799
1B-2_89	0.0445	0.1285	4.6788	2.1867	0.3447	0.2585	8.8338	0.4774	2.5234	1.9449	6.3323	0.6501	0.2585	0.4108
3B-10_89	0.0000	0.1725	2.8613	1.7602	1.0084	0.8945	8.0503	0.3135	12.0888	9.6453	8.3372	1.8236	1.2180	3.2610
2A-16_89	0.0000	0.6793	9.2079	6.0568	3.5476	3.0561	0.0000	0.0000	0.0134	0.6104	0.0513	0.4316	0.8107	5.0235
3B-13_87	0.0000	0.6132	6.1959	3.6575	2.1715	2.1896	0.9380	0.0109	3.5288	6.3833	5.2543	2.9384	2.4230	5.0596
2C-3_89	0.0000	0.0945	1.9816	1.2499	0.6847	0.6148	12.0544	0.7078	13.1206	8.3103	6.9318	1.4075	0.9537	2.3352
4A-13_87	0.0663	0.0770	3.8635	2.0619	0.5211	0.3708	1.7265	0.0281	7.9177	7.0769	8.5846	3.6462	3.0240	5.1924
3C-7_87	0.0000	0.3042	3.3510	1.9435	1.1440	1.0161	11.5675	0.7600	10.9379	7.8186	9.1547	2.8085	1.8631	3.3501
2C-9_89	0.0000	0.1272	2.0001	1.2072	0.6857	0.5938	9.7225	0.3462	12.5022	9.2339	6.7779	1.6329	1.0698	2.7763
3B-16_89	0.0000	0.7923	10.9409	7.2913	4.4541	4.0673	0.0000	0.0000	0.0482	0.7304	0.1012	0.5204	0.8556	5.0495
3A-16_87	0.0000	1.0800	10.1746	6.2457	3.7233	3.8651	0.0158	0.0000	0.0923	1.1428	0.4038	1.0425	1.4971	4.5043
3C-7_87	0.0000	0.3102	3.3675	1.9425	1.1428	1.0223	11.6399	0.7610	11.0177	7.8843	9.2055	2.8173	1.8434	3.3382
3B-2_87	0.0000	0.2252	2.4409	1.4447	0.8103	0.7547	12.2616	0.8940	9.8246	6.3975	7.5586	2.2041	1.4689	2.6550
2C-16_87	0.0000	0.8364	14.1904	9.1544	5.7421	5.7287	0.0000	0.0000	0.0275	0.7077	0.2429	0.7682	1.2524	4.4717
2A-6_87	0.0000	0.2147	4.6615	2.9188	1.7979	1.5575	8.3659	0.5778	8.2317	6.4467	7.7726	2.3569	1.6647	3.1671
1B-6_89	0.0560	0.1713	6.0835	2.8443	0.4833	0.3620	8.3989	0.4514	2.9437	2.3689	7.5755	0.8078	0.3480	0.5409
1C-10_87	0.0556	0.2018	9.8469	4.6863	0.6977	0.5664	6.6935	0.2224	3.4208	3.6486	0.8078	1.2279	0.5395	0.8456
3A-10_87	0.0000	0.3480	3.7174	2.1694	1.2609	1.1427	8.5467	0.4792	9.9798	7.9092	8.7850	2.8738	1.9485	3.5723

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
3B-1_89	0.0000	0.1180	1.6363	0.9739	0.5660	0.4926	12.3159	0.6856	13.3224	8.2090	7.6978	1.4224	0.9180	2.2654
2B-8_89	0.0000	0.1370	2.1346	1.3226	0.7662	0.6139	10.9998	0.4051	14.8579	10.1296	7.4228	1.7792	1.1780	3.0360
4C-16_87	0.1650	0.1877	8.2069	4.4994	1.2244	0.8455	0.0168	0.0000	0.1152	1.4794	0.6921	1.6024	2.3223	6.1131
1B-12_87	0.0758	0.2367	10.6831	5.0381	0.8172	0.6313	4.6194	0.1236	2.9200	3.6682	0.7757	1.3371	0.5824	0.9368
2A-5_89	0.0000	0.1076	1.9381	1.2214	0.6981	0.6130	12.1890	0.5869	14.5183	9.1663	7.2429	1.5669	1.1246	2.7124
4A-11_87	0.0413	0.0496	2.5955	1.3600	0.3455	0.2376	6.2649	0.3449	8.8683	7.5530	11.4559	3.3662	2.4885	3.9930
2C-17_87	0.0000	1.1413	20.3434	14.1403	9.1213	8.2120	0.0000	0.0000	0.0000	0.0240	0.0000	0.0643	0.4214	2.5296
3B-15_89	0.0000	0.5497	7.4471	4.8992	2.9103	2.6134	0.0676	0.0000	0.9770	4.2695	1.5558	1.5305	1.6039	6.0319
3C-5_89	0.0000	0.1309	1.8765	1.1190	0.6354	0.5743	12.2029	0.6323	13.8061	8.9814	8.2490	1.5684	0.9941	2.5516
4C-18_87	0.3758	0.5972	16.1252	10.6004	3.1051	2.2923	0.0142	0.0000	0.0073	0.0000	0.0000	0.0072	0.1076	1.2596
2B-9_89	0.0000	0.1420	2.0327	1.2620	0.7138	0.6219	10.1313	0.3286	14.1847	10.1871	7.0620	1.7313	1.1736	2.9400
1B-1_87	0.0337	0.1325	6.5785	3.2019	0.4671	0.3833	8.4631	0.3234	2.8334	2.4207	0.5472	0.7736	0.2418	0.4864
2A-1_89	0.0000	0.0830	1.7351	1.1272	0.6215	0.5626	11.4101	0.6401	12.1820	7.7374	6.2370	1.3235	0.8332	2.1903
3B-7_87	0.0000	0.3051	3.2763	1.8931	1.1056	0.9938	11.3713	0.7397	10.8874	7.7725	9.0169	2.7814	1.8169	3.2922
2A-4_89	0.0000	0.1084	1.7395	1.0886	0.6263	0.5312	12.7485	0.5937	14.4937	8.9913	7.0181	1.5168	0.9987	2.4874
3A-14_87	0.0000	0.6287	6.3172	3.7548	2.2522	2.2527	0.4660	0.0000	2.2792	5.1666	3.8906	2.5535	2.2273	4.8312
2C-1_89	0.0000	0.0892	1.6365	1.0168	0.5756	0.4986	11.6770	0.6195	12.6006	7.8106	6.1688	1.3327	0.8632	2.1564
3B-8_87	0.0000	0.3297	3.4988	2.0707	1.1703	1.1269	10.4561	0.6449	10.6747	7.8771	8.9832	2.8548	1.8874	3.4279
3C-16_87	0.0000	1.2046	10.8088	6.7490	4.0319	4.1011	0.0143	0.0000	0.0226	0.4143	0.1115	0.5312	1.0249	3.6986

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2A-5_87	0.0000	0.1906	4.1545	2.6167	1.5992	1.3365	9.0533	0.6959	8.0582	6.0813	7.5287	2.1800	1.5520	2.8161
4A-18_87	0.4459	0.8642	18.7940	13.6838	3.9807	3.1768	0.0161	0.0000	0.0075	0.0056	0.0000	0.0680	0.0594	0.3734
3C-8_87	0.0000	0.3116	3.3537	1.9867	1.1145	1.0367	10.1822	0.6291	10.4172	7.6283	8.6616	2.7201	1.8162	3.3134
2C-2_89	0.0000	0.0929	1.6636	1.0317	0.5851	0.5115	11.7569	0.5923	12.3463	7.9847	6.5043	1.3698	0.8832	2.2002
3B-14_89	0.0000	0.4312	5.8360	3.6569	2.1622	1.9246	0.5111	0.0000	3.3387	7.5132	3.7578	2.0070	1.7302	5.7438
1C-16_87	0.1606	0.5789	24.6482	12.6323	2.0648	1.6522	0.0000	0.0000	0.0000	0.0960	0.0000	0.1363	0.1346	0.6284
1A-9_87	0.0618	0.1822	9.0994	4.2716	0.6767	0.5042	7.4984	0.2675	3.4915	3.5464	0.8055	1.1916	0.4990	0.8034
3B-9_89	0.0000	0.1675	2.5395	1.5451	0.9121	0.7723	10.1610	0.4181	14.0515	10.1510	8.9138	1.8456	1.2359	3.2059
4C-6_87	0.0282	0.0330	1.8421	0.9572	0.2405	0.1594	9.9328	0.8137	9.7922	6.6386	11.1337	2.7847	1.9439	2.9699
1C-3_87	0.0563	0.1268	3.9187	1.7452	0.2767	0.1964	11.0893	0.4195	3.8183	2.9053	0.6226	0.9149	0.3652	0.5278
2C-2_87	0.0019	0.1683	3.2398	2.0372	1.2348	1.0773	10.8922	0.8487	8.4255	5.8749	7.1568	2.1037	1.4208	2.5554
2C-17_89	0.0000	1.0649	12.2417	8.8075	5.4461	4.9551	0.0000	0.0000	0.0000	0.0054	0.0000	0.0235	0.1312	2.1639
2B-16_89	0.0019	0.8473	9.3812	6.1647	3.6005	3.1495	0.0108	0.0000	0.0072	0.1995	0.0151	0.2080	0.4930	3.8456
1B-11_87	0.0752	0.2162	9.8394	4.6371	0.7224	0.5637	5.7973	0.1750	3.2701	3.7184	0.8066	1.3209	0.5453	0.9007
1C-5_89	0.0490	0.1512	6.2005	2.9212	0.5026	0.3731	7.9479	0.4749	2.6293	2.1416	6.9972	0.7382	0.2861	0.4857
1C-9_89	0.0297	0.1898	9.4595	4.6579	0.7245	0.5956	7.5183	0.4812	2.5928	2.3698	8.5110	0.7423	0.3326	0.6104
3C-15_89	0.0000	0.4601	6.8922	4.3522	2.5993	2.3299	0.2226	0.0000	2.0367	6.1576	2.7018	1.8413	1.7082	5.9572
4B-10_87	0.0361	0.0432	2.2932	1.2093	0.2991	0.2169	7.3676	0.4641	19.7233	7.2821	11.4457	3.1795	2.3279	3.6225
4A-3_87	0.0255	0.0305	1.6312	0.8403	0.2141	0.1484	10.1943	0.9030	19.4028	6.1172	10.3953	2.5323	1.7854	2.7234

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2B-18_89	0.0000	1.7884	12.7892	11.4727	7.8896	8.3217	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2154
3A-14_87	0.0000	0.6341	6.3019	3.7624	2.2287	2.1659	0.4797	0.0000	2.2405	5.1106	3.8625	2.5508	2.1872	4.7778
2C-9_87	0.0000	0.2715	4.8941	2.9951	1.7947	1.4753	8.1731	0.4749	9.1303	7.5675	8.7381	2.7782	1.9566	3.7170
3B-8_89	0.0000	0.1551	2.4434	1.4931	0.8836	0.7995	10.1781	0.4554	13.4824	9.5919	8.4584	1.7347	1.1413	3.0002
2C-2_89	0.0000	0.0964	1.6720	1.0319	0.6038	0.5278	12.0840	0.5897	12.4347	8.1320	6.4973	1.3862	0.8954	2.2847
3C-7_87	0.0000	0.3115	3.3365	1.9263	1.1329	1.0673	11.6244	0.7533	11.0639	7.8798	9.0577	2.8268	1.8538	3.3814
1B-19_87	0.2169	1.1865	48.0006	29.0750	5.2291	4.4921	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0978
1B-7_89	0.0477	0.1742	7.8481	3.7697	0.6049	0.4893	7.4062	0.4596	2.6453	2.3543	7.8681	0.8174	0.3090	0.5568
2B-5_89	0.0000	0.1165	1.8659	1.1479	0.6649	0.5481	12.0726	0.5201	14.0370	8.8595	6.8274	1.5200	1.0051	2.5434
3C-19_89	0.0000	1.8581	13.9760	11.6804	7.9819	8.0429	0.0000	0.0000	0.0000	0.0000	0.0000	0.0387	0.1251	0.4560
4C-11_87	0.0248	0.0419	2.3811	1.2386	0.3117	0.1991	6.5918	0.3560	16.7646	7.4965	11.2316	3.3059	2.4474	3.8564
3C-1_87	0.0000	0.1980	2.1505	1.2564	0.7084	0.6579	11.9180	0.8925	9.0386	5.7061	6.8529	1.9855	1.3158	2.2857
2C-9_87	0.0000	0.2756	4.7298	2.9171	1.7192	1.4490	8.1784	0.4722	9.1419	7.5917	8.6194	2.7623	1.9385	3.4527
2A-17_87	0.0000	1.1562	18.3832	12.8447	8.2741	7.3536	0.0000	0.0000	0.0052	0.0238	0.0000	0.0673	0.3812	2.4436
4C-9_87	0.0322	0.0383	2.1955	1.1157	0.2800	0.1853	8.9627	0.6495	18.3661	7.5593	12.1197	3.1895	2.3133	3.5794
4B-5_87	0.0261	0.0311	1.7533	0.9112	0.2338	0.1542	10.1634	0.8752	9.6634	6.3891	10.9131	2.6721	1.8813	2.8355
3C-7_89	0.0000	0.1452	2.1107	1.2815	0.7621	0.6775	10.8413	0.5069	13.3509	9.1938	8.3313	1.6464	1.0864	2.7672
2B-6_89	0.0000	0.1182	2.0642	1.2980	0.7425	0.6170	11.3070	0.4860	14.0950	9.3270	7.2583	1.6246	1.0855	2.7839
3C-9_87	0.0000	0.3180	3.4079	1.9835	1.1711	1.0547	9.3730	0.5526	10.0354	7.5906	8.5060	2.7004	1.8378	3.3416

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
4B-14_87	0.2094	0.2845	10.6607	6.1109	1.6213	1.1914	0.0301	0.0000	0.0899	0.3338	0.2034	0.5001	1.1629	4.3152
1A-2_89	0.0331	0.1234	4.9057	2.3033	0.3608	0.2769	7.9611	0.4844	2.4000	1.8915	6.2599	0.6100	0.2335	0.4057
2C-5_89	0.0000	0.1135	1.8535	1.1491	0.6600	0.5367	12.7161	0.5658	14.7120	9.2620	7.1589	1.5849	1.0273	2.6428
1A-13_89	0.0781	0.3062	14.1283	6.9741	1.1615	0.9643	0.6997	0.0217	0.7861	1.7960	5.5988	0.7641	0.3832	0.7282
1B-5_87	0.0540	0.1379	5.8545	2.6955	0.4273	0.3186	9.5290	0.3616	3.6238	3.0592	0.7002	1.0035	0.4055	0.6190
4B-12_87	0.0398	0.0502	2.6043	1.3651	0.3401	0.2328	5.5920	0.2672	15.6563	7.4988	11.0164	3.3676	2.5260	4.0397
4A-6_87	0.0268	0.0347	1.8572	0.9683	0.2439	0.1658	9.8775	0.8145	19.8950	6.6615	11.1451	2.8010	1.9937	3.0705
2B-5_87	0.0000	0.1711	4.6376	3.0438	1.8052	1.6897	11.1788	1.0543	8.6955	6.1852	8.4709	2.3761	1.5544	2.8638
1C-7_87	0.0615	0.1596	6.6965	3.0844	0.4828	0.3680	9.3133	0.3463	3.8584	3.4778	0.7769	1.1302	0.4670	0.7020
2B-13_89	0.0000	0.3180	4.6290	2.8552	1.6420	1.3944	1.4405	0.0038	6.2163	9.4367	4.5864	2.1562	1.8871	5.2857
3C-13_89	0.0000	0.3096	4.5704	2.8115	1.6529	1.4557	2.6494	0.0282	8.0390	9.9787	6.8230	2.1654	1.6406	4.8492
3A-2_87	0.0000	0.2367	2.5214	1.4944	0.8377	0.7788	12.9148	0.9440	10.2498	6.6024	7.8054	2.3085	1.5501	2.6888
1B-7_87	0.0422	0.1444	7.8227	3.6832	0.5169	0.4173	9.3102	0.3911	3.5798	3.2341	0.7628	1.0477	0.3791	0.6574
3C-6_87	0.0000	0.2910	3.1261	1.8099	1.0620	0.8986	11.9870	0.8076	10.8329	7.5384	8.8124	2.6745	1.7659	3.1504
3C-19_89	0.0000	1.8451	14.5889	12.2413	8.3563	8.6288	0.0061	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4145
3A-8_87	0.0000	0.3317	3.3828	2.0138	1.1551	1.1676	11.2008	0.6953	11.0205	7.9840	8.9115	2.8533	1.9217	3.2365
3A-8_89	0.0000	0.1439	2.0895	1.2424	0.7352	0.6498	8.9777	0.3797	12.1140	8.6056	7.6040	1.5632	1.0328	2.7102
1B-5_89	0.0453	0.1573	6.4719	3.0898	0.4959	0.3856	7.8891	0.4664	2.6333	2.1658	7.1769	0.7216	0.2962	0.4910
2A-13_89	0.0000	0.2861	4.7907	2.9479	1.6918	1.4427	1.5041	0.0000	6.1902	9.5755	4.7729	2.1426	1.7671	5.4147

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
1B-10_89	0.0696	0.2281	9.3961	4.4726	0.7462	0.5848	5.3956	0.2882	2.4691	2.5882	8.3233	0.9270	0.3766	0.6648
3A-16_87	0.0000	1.0851	10.2405	6.2960	3.7027	3.7405	0.0166	0.0000	0.0910	1.1378	0.4084	1.0460	1.4721	4.5177
3C-2_89	0.0000	0.1166	1.5494	0.9147	0.5209	0.4665	11.3391	0.6171	12.3081	7.7165	7.2238	1.3305	0.8415	2.1667
2A-14_89	0.0000	0.3861	8.0144	5.0764	2.9455	2.7063	0.2079	0.0000	1.9757	6.1089	2.3138	1.7726	1.6664	6.2527
2A-4_87	0.0000	0.1780	3.5664	2.2647	1.3414	1.1296	10.6881	0.8334	8.8881	6.3275	7.7089	2.3380	1.5777	2.6983
2B-19_87	0.0000	3.0606	21.5623	25.4390	19.7284	24.3993	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3B-11_89	0.0000	0.1997	3.2336	1.9780	1.1683	1.0435	7.1573	0.2204	12.6110	10.4076	8.6059	2.0063	1.4242	3.7196
3A-18_89	0.0000	1.3330	13.0193	9.6686	6.1833	5.7100	0.0000	0.0000	0.0000	0.0024	0.0000	0.0176	0.0686	1.6466
4C-2_87	0.0198	0.0272	1.5798	0.8096	0.2054	0.1344	10.2198	0.9375	19.5639	5.9455	10.3434	2.4678	1.7352	2.5926
4C-17_87	0.2609	0.3375	11.8510	6.9668	1.9309	1.3611	0.0172	0.0000	0.0065	0.0828	0.0122	0.2603	0.8302	3.7641
1C-3_89	0.0423	0.1386	5.2731	2.4970	0.4043	0.3127	8.1391	0.4756	2.5577	1.9833	6.6227	0.6635	0.2619	0.4409
4C-6_87	0.0278	0.0323	1.8549	0.9594	0.2477	0.1612	9.9346	0.8172	20.9148	6.6610	11.1877	2.7956	1.9412	2.9948
4B-8_87	0.0329	0.0360	2.0337	1.0539	0.2723	0.1806	9.0145	0.6807	20.5618	7.0016	11.5206	2.9907	2.1458	3.2637
3B-16_89	0.0000	0.7915	10.1169	6.9558	4.2411	3.8603	0.0000	0.0000	0.0357	0.7422	0.1039	0.5325	0.9018	5.0984
2C-7_87	0.0000	0.2231	4.4452	2.7669	1.6838	1.3783	9.1598	0.6346	8.9332	6.9299	8.1230	2.5374	1.7030	3.1846
3C-14_87	0.0000	0.6639	6.6030	3.9273	2.3365	2.3512	0.3943	0.0000	2.0296	5.0126	3.7307	2.5274	2.2054	4.9586
1C-17_89	0.1864	0.8856	42.1195	24.3309	4.3978	3.7844	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1872
4A-5_87	0.0268	0.0313	1.7443	0.8996	0.2275	0.1597	10.2046	0.8703	9.7105	6.4753	10.8863	2.7044	1.9045	2.9142
3C-18_87	0.0000	2.3883	14.8423	11.0937	7.2392	7.5484	0.0149	0.0000	0.0075	0.0000	0.0000	0.0000	0.0054	0.4098

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
4A-12_87	0.0449	0.0520	2.7619	1.4569	0.3710	0.2575	5.4798	0.2515	15.6047	7.7266	11.2414	3.4974	2.6279	4.1682
1B-15_87	0.1071	0.3647	18.1653	8.9448	1.4581	1.1120	0.0489	0.0000	0.1647	1.1661	0.1819	0.6657	0.4142	0.9270
3B-9_87	0.0000	0.3539	3.7335	2.1403	1.2846	1.1447	10.2770	0.6022	11.0426	8.4529	9.4369	3.0672	2.0283	3.7059
4C-8_87	0.0276	0.0352	2.0586	1.0635	0.2651	0.1766	9.3321	0.6904	10.1224	7.2272	11.7395	3.0661	2.1857	3.4290
4B-1_87	0.0161	0.0255	1.4879	0.7636	0.1939	0.1332	10.0210	0.9380	18.8232	5.6047	9.7957	2.3143	1.6192	2.4754
3A-10_89	0.0000	0.1806	2.8556	1.7468	1.0336	0.9161	8.3051	0.2997	12.9970	10.0725	8.5292	1.8840	1.2620	3.3690
1B-7_87	0.0664	0.1593	6.6206	3.0426	0.4661	0.3548	9.2242	0.3295	3.9080	3.4840	0.7701	1.1209	0.4218	0.6944
2B-8_89	0.0000	0.1420	2.1204	1.2850	0.7259	0.6371	11.1122	0.3952	14.8147	10.2203	7.3698	1.7511	1.2070	2.9638
3B-17_87	0.0000	1.8965	13.9834	9.7973	6.0323	6.1647	0.0115	0.0000	0.0079	0.0000	0.0000	0.0108	0.1333	1.1849
2C-4_89	0.0000	0.1163	1.6623	1.0033	0.5743	0.4895	13.2996	0.6241	15.1083	9.3703	7.1142	1.5465	1.0247	2.4426
2B-6_89	0.0000	0.1202	2.0508	1.2977	0.7384	0.6573	11.2607	0.4817	14.0241	9.2680	7.2857	1.6122	1.0653	2.7355
3B-6_87	0.0000	0.2875	3.0210	1.7555	1.0379	0.9356	11.3735	0.7707	10.2603	7.0939	8.3380	2.5440	1.6704	3.0037
1A-5_89	0.0408	0.1477	6.3944	3.0642	0.5093	0.3815	7.6946	0.4978	2.5216	2.0864	7.0999	0.7118	0.2800	0.4692
4B-16_87	0.3394	0.5594	15.9473	10.2927	2.8651	2.1820	0.0217	0.0000	0.0065	0.0276	0.0150	0.0441	0.2069	1.4991
2B-17_87	0.0000	1.3366	24.3696	18.0413	11.8848	11.6657	0.0000	0.0000	0.0000	0.0000	0.0000	0.0100	0.1038	1.5366
4B-9_87	0.0302	0.0412	2.1166	1.0914	0.2744	0.1944	8.5868	0.6176	20.2017	7.1052	11.5394	3.0344	2.1913	3.4082
2B-15_89	0.0000	0.5174	7.5738	5.0005	2.8796	2.5379	0.0188	0.0000	0.4387	2.7084	0.6401	1.1190	1.3564	5.8693
4A-2_87	0.0237	0.0287	1.5848	0.8197	0.2104	0.1456	10.1456	0.9171	18.7501	5.8914	10.1299	2.4517	1.7368	2.6516
1A-14_87	0.1341	0.3565	13.2358	6.2904	1.0054	0.7753	0.1085	0.0000	0.3155	1.5485	0.2528	0.8449	0.4884	0.9391

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2B-13_87	0.0000	0.4611	8.5242	5.4489	3.2941	2.7877	0.6256	0.0000	2.4653	5.1783	4.3648	2.5064	2.1941	4.6782
3B-11_87	0.0000	0.4111	4.2214	2.4689	1.4763	1.3322	5.7404	0.2824	9.2838	8.3424	8.6880	3.1253	2.1904	4.0871
1C-10_89	0.0604	0.2142	9.4012	4.5401	0.7596	0.5745	5.6861	0.3449	2.4681	2.4938	8.2980	0.9072	0.3708	0.6494
2B-7_87	0.0000	0.2175	5.4433	3.7209	2.1680	1.9120	9.4224	0.7971	8.5242	6.6387	8.6753	2.5625	1.7500	3.2315
2B-4_87	0.0000	0.2053	3.8682	2.4175	1.4828	1.1823	10.2708	0.7577	8.9719	6.5608	7.8201	2.3464	1.6499	2.8548
1C-7_87	0.0391	0.1543	7.7270	3.6530	0.5347	0.3937	9.2574	0.3954	3.6404	3.2805	0.7879	1.0417	0.3745	0.6457
1C-4_89	0.0188	0.1302	6.5040	3.1527	0.5059	0.3809	8.7838	0.6148	2.4819	2.0186	7.1315	0.6257	0.2381	0.4398
3A-10_87	0.0000	0.3489	3.7286	2.1768	1.2898	1.1851	8.5807	0.4721	9.9365	7.9330	8.8476	2.9083	1.9417	3.5896
4A-14_87	0.0812	0.0943	4.6682	2.5056	0.6357	0.4561	0.4768	0.0000	3.4667	5.5242	5.4711	3.3256	3.0568	5.7054
2C-10_89	0.0000	0.1516	2.2616	1.4084	0.7987	0.6741	9.0732	0.2749	13.8862	10.3173	7.1870	1.8116	1.2588	3.1331
1A-3_87	0.0642	0.1293	4.0707	1.8136	0.2898	0.2017	11.4584	0.4282	3.9653	3.0279	0.6485	0.9460	0.3692	0.5633
3C-19_87	0.0000	3.8253	12.3268	12.6395	9.3754	11.2159	0.0117	0.0000	0.0053	0.0000	0.0000	0.0000	0.0000	0.0088
3B-18_89	0.0000	1.8173	13.2913	11.0292	7.5216	7.2771	0.0057	0.0000	0.0000	0.0019	0.0000	0.0000	0.0000	0.5275
4C-15_87	0.1094	0.1193	5.6979	3.0475	0.8173	0.5573	0.1583	0.0000	1.6999	4.4252	3.6817	3.0012	3.0554	6.1964
1B-7_89	0.0429	0.1727	7.8253	3.7785	0.6087	0.4622	7.7365	0.4941	2.6701	2.3203	8.0073	0.7828	0.3092	0.5332
3A-18_87	0.0000	2.0431	14.5847	10.3195	6.5757	6.7872	0.0093	0.0000	0.0087	0.0000	0.0000	0.0000	0.0337	0.8521
4A-1_87	0.0208	0.0226	1.4874	0.7673	0.1898	0.1256	10.3211	0.9397	8.9732	5.7467	9.7534	2.3585	1.6659	2.5241
1B-11_89	0.0839	0.2517	10.2606	4.9066	0.8374	0.6481	3.8138	0.1866	2.1625	2.5658	8.0517	0.9599	0.4298	0.7158
1B-2_89	0.0324	0.1277	5.2001	2.4783	0.3808	0.3050	7.9837	0.4828	2.4332	1.8956	6.2977	0.6140	0.2426	0.4079

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
3A-17_87	0.0000	1.2524	11.2963	7.1178	4.2257	4.2452	0.0178	0.0000	0.0107	0.2754	0.0491	0.4052	0.8601	3.5723
2C-6_87	0.0000	0.2061	4.1568	2.6713	1.6313	1.4347	10.6409	0.8157	9.2745	6.7949	8.1800	2.4412	1.6393	2.9896
3C-1_89	0.0000	0.1149	1.6106	0.9572	0.5513	0.4878	11.7144	0.6688	12.5383	7.8555	7.4763	1.3589	0.8637	2.1946
4C-1_87	0.0197	0.0257	1.4051	0.7248	0.1777	0.1158	9.8364	0.9205	8.5440	5.4347	9.4156	2.2499	1.5881	2.3401
1C-11_89	0.0776	0.2482	10.5264	5.0534	0.8609	0.6573	4.0647	0.2089	2.1695	2.5430	8.0767	0.9266	0.4151	0.6945
1B-11_87	0.0884	0.2231	8.4591	3.9170	0.6184	0.4731	6.0891	0.1716	3.5599	3.9461	0.8126	1.3680	0.5973	0.9088
2A-7_87	0.0000	0.2377	4.1460	2.5236	1.5037	1.2292	9.0543	0.5590	9.2063	7.0308	8.2160	2.5401	1.8057	3.1636
2B-6_87	0.0000	0.2065	4.7670	3.0520	1.7959	1.6234	9.6560	0.7125	8.7832	6.6706	8.2446	2.4699	1.6273	3.0447
1A-9_87	0.0321	0.1746	10.3732	5.0038	0.7405	0.5803	7.7312	0.3408	3.3761	3.3809	0.8269	1.0999	0.4248	0.7758
1C-13_89	0.1331	0.3565	11.5893	5.5095	0.9423	0.7232	0.6104	0.0163	0.8249	1.9419	5.1943	0.8594	0.4446	0.8159
2A-10_87	0.0000	0.2736	5.3754	3.3677	2.0871	1.6793	6.8555	0.3978	8.3960	7.3349	8.4186	2.7807	1.9503	3.6816
1C-18_87	0.3315	1.4724	42.0768	25.5872	4.5870	3.9167	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0570
1A-16_87	0.1575	0.5297	23.4525	12.0306	2.0237	1.5657	0.0000	0.0000	0.0000	0.1272	0.0160	0.1677	0.1284	0.5675
2C-6_89	0.0000	0.1102	1.9894	1.2659	0.7318	0.6577	10.7306	0.4762	13.4143	8.7377	6.8205	1.5202	1.0093	2.5715
1C-13_87	0.1141	0.3247	13.2354	6.3178	1.0197	0.7759	0.5965	0.0044	0.9044	2.4595	0.4445	1.1121	0.5803	1.0231
1A-12_89	0.0810	0.2547	10.4487	5.0035	0.8490	0.6668	3.6002	0.1637	2.1332	2.5860	7.9330	0.9644	0.4415	0.7228
3A-11_87	0.0000	0.3904	4.0955	2.3842	1.4283	1.2971	6.2086	0.3323	9.4478	8.2005	8.7214	3.0435	2.1177	3.9093
4B-13_87	0.0653	0.0723	3.6656	1.9560	0.5000	0.3473	2.1704	0.0432	9.1237	7.4270	9.1453	3.7345	3.0467	5.1606
1A-6_87	0.0178	0.1383	7.1899	3.4196	0.5002	0.3745	10.0187	0.4183	3.6661	3.1926	0.7516	0.9892	0.3366	0.6193

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
3B-10_89	0.0000	0.1799	2.6824	1.6377	0.9592	0.8348	8.2790	0.2996	12.1219	9.8121	8.3971	1.8347	1.2314	3.2675
2B-4_87	0.0000	0.1903	4.0064	2.6013	1.5290	1.2952	11.3489	0.9420	9.0398	6.3978	8.1616	2.3401	1.5757	2.7982
2C-13_87	0.0000	0.4127	7.4364	4.6932	2.8284	2.3969	1.1931	0.0234	3.7348	6.0608	5.4616	2.6927	2.1928	4.5683
2A-12_87	0.0000	0.3158	7.3514	4.7396	2.9172	2.4214	4.0321	0.1889	6.5471	6.9712	7.8973	2.7988	2.1082	4.0375
3A-13_87	0.0000	0.5616	5.8052	3.3946	2.0110	1.9475	1.6317	0.0267	4.7077	7.0195	6.0924	3.0454	2.4048	4.7385
2B-17_89	0.0000	1.1891	11.6190	8.3103	5.1335	4.6468	0.0062	0.0000	0.0000	0.0034	0.0000	0.0128	0.0886	1.8018
1A-17_89	0.1711	0.6084	25.6341	13.4133	2.3764	1.9047	0.0000	0.0000	0.0000	0.0660	0.1240	0.0966	0.0830	0.4787
2B-19_87	0.0000	3.0799	19.7316	22.7376	17.2828	21.5536	0.0047	0.0000	0.0053	0.0000	0.0000	0.0000	0.0000	0.0000
2C-10_89	0.0000	0.1479	2.4854	1.5657	0.9004	0.7522	8.6092	0.2620	13.3299	9.9436	7.2059	1.7909	1.2508	3.2648
1B-11_87	0.0900	0.2275	8.4512	3.8959	0.6111	0.4549	6.0080	0.1651	3.4820	3.9124	0.8179	1.3481	0.5778	0.8996
2A-4_89	0.0000	0.1028	2.0342	1.2867	0.7455	0.6631	11.6320	0.5884	14.1327	8.7514	6.8669	1.4676	1.0513	2.6379
2B-10_89	0.0000	0.1560	2.3114	1.4510	0.8199	0.6795	8.3481	0.2317	13.2827	10.1245	6.9209	1.7951	1.2562	3.1683
1A-9_89	0.0636	0.2026	7.7188	3.6502	0.6118	0.4789	6.9705	0.3808	2.8398	2.5542	8.0372	0.8886	0.3838	0.6053
2C-11_87	0.0000	0.3150	5.1330	3.1501	1.8735	1.5273	5.0561	0.2507	7.9981	7.5724	8.1269	2.8768	2.0835	3.7520
1A-14_87	0.1497	0.3656	12.3845	5.8477	0.9323	0.7030	0.1173	0.0000	0.3143	1.5910	0.2536	0.8397	0.4719	0.9498
4C-6_87	0.0271	0.0331	1.8370	0.9537	0.2490	0.1568	9.9570	0.8211	21.4320	6.6671	11.1543	2.8005	1.9585	2.9957
2A-12_89	0.0000	0.1916	3.1616	1.9966	1.1442	0.9673	5.9033	0.1077	12.0393	10.7731	6.9993	2.0640	1.5130	4.0658
4C-5_87	0.0222	0.0300	1.7622	0.9125	0.2318	0.1546	9.9985	0.8693	19.9394	6.3677	10.8706	2.6505	1.8732	2.8147
3C-6_87	0.0000	0.2900	3.0899	1.7940	1.0475	0.9376	12.0519	0.8120	10.7880	7.5499	8.7275	2.6583	1.7507	3.1534

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2C-1_87	0.0000	0.1360	2.7466	1.7575	1.0366	0.9227	10.6506	0.8665	7.8212	5.2881	6.5086	1.8362	1.2400	2.1538
3A-19_89	0.0000	1.9140	14.2216	12.4095	8.6835	9.1912	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3866
1A-19_89	0.2695	1.2361	38.7340	22.7777	4.1901	3.6020	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0890
2C-15_87	0.0000	0.6251	12.7507	8.5773	5.2911	4.5992	0.0130	0.0000	0.3841	2.1853	1.2999	1.5943	1.8698	4.8166
3C-16_87	0.0000	1.2068	10.8500	6.7827	4.0114	3.9967	0.0150	0.0000	0.0174	0.4208	0.1090	0.5264	0.9866	3.9067
1C-11_87	0.0665	0.2144	10.1027	4.7611	0.7601	0.5752	5.5552	0.1617	3.1516	3.6907	0.7985	1.3170	0.5670	0.9031
3A-9_89	0.0000	0.1643	2.5791	1.5848	0.9406	0.8509	8.8464	0.3591	12.7453	9.5742	8.2439	1.7537	1.1557	3.1067
2C-15_87	0.0000	0.6558	12.0049	7.7681	4.7632	4.0757	0.0406	0.0000	0.3701	2.2249	1.2776	1.5864	1.8547	4.8316
2A-7_89	0.0000	0.1179	2.0799	1.3206	0.7619	0.6816	10.9267	0.4709	13.3815	9.3398	7.1819	1.6170	1.0846	2.7776
4A-3_87	0.0291	0.0295	1.6267	0.8360	0.2101	0.1473	10.2091	0.8978	9.2398	6.1280	10.3504	2.5572	1.7987	2.7837
3B-9_89	0.0000	0.1700	2.4136	1.5114	0.8950	0.7429	10.2453	0.4165	14.0481	10.0856	8.9309	1.8534	1.2534	3.1026
1C-8_89	0.0666	0.1995	7.3581	3.4672	0.5847	0.4480	7.6037	0.4174	2.9778	2.6053	7.9969	0.8952	0.3875	0.6072
2A-18_87	0.0000	1.7490	27.7869	22.1043	15.0740	15.7812	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5325
2A-18_87	0.0000	1.7739	24.7355	19.4473	13.1474	13.3204	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5318
1C-11_87	0.0740	0.2175	10.1994	4.8378	0.7591	0.5774	5.5714	0.1572	3.2015	3.7525	0.8049	1.3125	0.5942	0.8971
4A-16_87	0.1723	0.2090	8.5235	4.6702	1.2786	0.8980	0.0158	0.0000	0.0624	1.0376	0.4179	1.2905	2.0494	5.7613
1A-11_87	0.0563	0.2149	10.8824	5.1701	0.8204	0.6234	4.9606	0.1497	2.9143	3.5849	0.7821	1.3132	0.5356	0.8992
2B-12_87	0.0000	0.3447	8.3249	5.3397	3.2876	2.7872	3.2189	0.1377	5.9494	6.8643	7.7373	2.8584	2.1412	4.4155
3A-3_89	0.0000	0.1286	1.7876	1.0686	0.6180	0.4994	12.2855	0.6505	13.4141	8.5952	7.9781	1.5032	0.9450	2.4488

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2A-14_89	0.0000	0.3876	7.0167	4.4551	2.6063	2.2393	0.2624	0.0000	2.0802	6.1420	2.2789	1.8412	1.7970	6.2429
1C-1_89	0.0373	0.1150	4.3752	2.0560	0.3349	0.2561	8.0124	0.4473	2.2707	1.7350	5.8219	0.5787	0.2323	0.3656
1C-2_87	0.0460	0.1104	3.4985	1.5656	0.2288	0.1701	10.1364	0.3874	3.4194	2.5826	0.5574	0.8150	0.3251	0.4744
2A-9_89	0.0000	0.1362	2.0486	1.2782	0.7382	0.6470	9.8507	0.3401	14.0102	9.7133	7.0593	1.7029	1.1447	2.9268
3A-16_87	0.0000	1.0850	10.2305	6.2022	3.6565	3.6212	0.0116	0.0000	0.0975	1.1276	0.4172	1.0311	1.4806	4.5569
1A-17_87	0.2261	0.7240	24.2713	12.6722	2.1060	1.6776	0.0000	0.0000	0.0000	0.0088	0.0000	0.0470	0.0691	0.4155
1C-2_87	0.0521	0.1117	3.4605	1.5430	0.2478	0.1743	10.0390	0.3856	3.4065	2.5800	0.5489	0.8040	0.3216	0.4689
2C-17_87	0.0000	1.1434	21.9496	15.4558	10.0102	8.9598	0.0000	0.0000	0.0000	0.0170	0.0000	0.0676	0.4133	2.5958
2B-14_89	0.0000	0.4253	6.2410	3.9174	2.2400	1.9553	0.2201	0.0000	2.1323	6.3285	2.2666	1.8111	1.7507	6.0227
3C-1_87	0.0000	0.1976	2.1058	1.2458	0.6968	0.6514	12.0949	0.8833	8.9504	5.7402	6.7981	1.9971	1.3171	2.2932
3B-16_89	0.0000	0.7939	10.1973	7.0051	4.2873	3.9137	0.0000	0.0000	0.0408	0.7418	0.1041	0.5453	0.8710	5.1410
3C-5_87	0.0000	0.2724	2.9395	1.6966	0.9928	0.8875	12.5556	0.8737	10.6631	7.2529	8.5858	2.5533	1.6777	2.9929
3B-6_89	0.0000	0.1404	1.9956	1.2141	0.6974	0.6293	11.0423	0.5456	13.2748	8.9186	8.0596	1.5708	1.0429	2.6288
4A-2_87	0.0229	0.0288	1.5741	0.8178	0.2052	0.1382	10.2380	0.9283	9.1227	5.9066	10.0790	2.4420	1.7132	2.6568
3A-13_89	0.0000	0.3239	4.8119	3.0100	1.7810	1.5651	2.0263	0.0170	7.0464	9.6244	6.1508	2.1579	1.6617	4.9815
3C-3_89	0.0000	0.1298	1.6375	0.9667	0.5535	0.4573	12.8911	0.6741	14.0672	8.7561	8.0685	1.5309	0.9848	2.4185
4B-8_87	0.0278	0.0354	2.0279	1.0505	0.2556	0.1831	9.0270	0.6731	21.0662	6.9769	11.4677	2.9694	2.1148	3.3253
1A-18_87	0.3797	1.1397	22.2371	12.0286	2.0424	1.5725	0.0058	0.0000	0.0079	0.0000	0.0000	0.0031	0.0019	0.1343
1A-10_87	0.0500	0.2010	11.5514	5.5591	0.8444	0.6773	5.9005	0.1997	3.0834	3.5068	0.8071	1.1892	0.4748	0.8483

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2B-1_89	0.0000	0.0930	1.7044	1.0820	0.6095	0.5292	11.5591	0.5852	12.6977	7.8858	6.4002	1.3431	0.8844	2.2730
1C-17_87	0.2273	0.8144	29.7046	16.0222	2.6933	2.2258	0.0000	0.0000	0.0000	0.0000	0.0000	0.0228	0.0232	0.2965
1C-12_89	0.0778	0.2630	10.7133	5.1958	0.8531	0.6805	3.1613	0.1486	1.9304	2.4912	7.7692	0.9616	0.4240	0.7188
2C-19_87	0.0000	2.1648	23.1786	20.5221	14.0655	15.7050	0.0000	0.0000	0.0053	0.0000	0.0000	0.0000	0.0000	0.0957
2B-5_87	0.0000	0.1962	4.0912	2.5027	1.5325	1.2515	9.0298	0.6508	8.5181	6.2870	7.9712	2.3354	1.6195	2.8978
1B-17_87	0.2016	0.6077	22.1751	11.2605	1.8550	1.4452	0.0000	0.0000	0.0050	0.0843	0.0101	0.1200	0.1398	0.5694
2A-10_89	0.0000	0.1452	2.3005	1.3740	0.7972	0.7020	9.1646	0.2713	12.8972	10.2118	7.1586	1.8256	1.2497	3.2273
1C-3_89	0.0359	0.1331	5.7680	2.7642	0.4434	0.3357	7.7557	0.5117	2.3421	1.9422	6.5129	0.6220	0.2377	0.4125
3C-7_89	0.0000	0.1440	2.2174	1.3391	0.7830	0.7101	10.3006	0.4868	12.9972	9.0751	8.2869	1.6288	1.0805	2.7728
1B-8_87	0.0242	0.1559	9.1747	4.3640	0.6705	0.5092	8.8460	0.3822	3.5318	3.3562	0.8041	1.0760	0.3904	0.7288
1A-3_89	0.0462	0.1576	6.2116	2.9663	0.4836	0.3804	7.6650	0.4306	2.4543	2.0308	6.3635	0.6670	0.2771	0.4690
1A-10_87	0.0530	0.1968	10.6236	5.0850	0.7779	0.6160	6.4002	0.2212	3.2074	3.5739	0.8060	1.2643	0.5142	0.8396
1B-2_87	0.0535	0.1122	3.5825	1.5926	0.2560	0.1833	10.7036	0.4054	3.5874	2.7443	0.5825	0.8509	0.3442	0.4820
2B-14_87	0.0000	0.5666	12.2799	8.1359	5.0240	4.2826	0.1044	0.0000	0.7858	3.1172	2.2092	1.9687	2.0398	5.0130
3A-7_87	0.0000	0.3098	3.1904	1.8739	1.1065	0.9925	11.3848	0.7591	10.6788	7.5398	8.8516	2.7031	1.7879	3.2051
3A-17_89	0.0000	0.9902	10.7538	7.4600	4.5710	4.0859	0.0056	0.0000	0.0069	0.1284	0.0113	0.1570	0.4251	3.7349
3A-10_89	0.0000	0.1861	2.7263	1.6515	0.9691	0.8738	8.5615	0.3008	13.1626	10.2366	8.6909	1.8842	1.2886	3.3761
2C-1_89	0.0000	0.0876	1.6214	1.0246	0.5906	0.5281	11.7988	0.6236	12.8225	7.8220	6.3301	1.3181	0.8648	2.2481
1B-13_87	0.1322	0.3182	11.2802	5.2690	0.8301	0.6221	1.1059	0.0129	1.3730	2.9219	0.5315	1.2359	0.5899	1.0361

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
3A-1_87	0.0000	0.1973	2.1087	1.2690	0.7009	0.6884	12.0125	0.9005	9.0484	5.7112	6.8153	2.0037	1.3094	2.1440
1C-11_87	0.0807	0.2267	9.3222	4.3259	0.6866	0.5192	5.5418	0.1560	3.3303	3.8110	0.8098	1.3497	0.5852	0.9098
3A-3_87	0.0000	0.2457	2.6049	1.5267	0.8991	0.8063	12.7854	0.9222	10.1907	6.7308	8.0351	2.3456	1.5389	2.7416
2C-1_87	0.0000	0.1438	2.9571	1.9001	1.0961	0.9219	9.9991	0.8461	7.5800	5.1837	6.5459	1.8656	1.2165	2.1031
2C-3_87	0.0000	0.1908	3.9609	2.4663	1.5036	1.2285	10.9122	0.8220	8.9810	6.3912	7.8440	2.3102	1.5273	2.7571
1C-18_89	0.3494	1.8978	47.5208	30.9706	5.8467	5.3001	0.0052	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0195
4A-9_87	0.0331	0.0408	2.2089	1.1596	0.3000	0.1990	8.6101	0.6094	21.0151	7.1577	11.5639	3.0713	2.2285	3.4244
4C-3_87	0.0228	0.0246	1.6499	0.8427	0.2159	0.1417	10.2970	0.9193	9.4627	6.1323	10.5614	2.5613	1.7954	2.6838
2A-11_87	0.0000	0.3157	4.9895	2.9931	1.7749	1.4465	5.5992	0.2447	8.0838	7.5120	7.9504	2.8398	2.0608	3.6625
3C-15_87	0.0000	0.8812	8.5519	5.1662	3.0101	3.0015	0.0398	0.0000	0.4036	2.4973	1.3669	1.6854	1.9208	4.6572
2A-8_87	0.0000	0.2503	4.3844	2.6897	1.6123	1.3367	8.6099	0.5225	9.0217	7.2483	8.3352	2.6386	1.8204	3.4444
4A-13_87	0.0659	0.0797	3.8029	2.0032	0.5164	0.3730	1.8208	0.0321	7.8227	7.1062	8.2072	3.6345	3.0383	5.2601
3B-12_89	0.0000	0.2145	3.2610	1.9959	1.1940	1.0202	6.0849	0.1474	11.2448	10.3591	7.9938	2.0101	1.4351	3.8834
1C-7_87	0.0579	0.1498	7.6306	3.6116	0.5290	0.3931	10.1083	0.4314	3.9252	3.0530	0.8041	1.0171	0.2922	0.5883
3C-18_87	0.0000	2.3813	14.8187	11.0653	7.2297	7.6941	0.0148	0.0000	0.0074	0.0000	0.0000	0.0000	0.0076	0.4148
3C-5_87	0.0000	0.2737	2.9374	1.6994	0.9862	0.9006	12.5433	0.8735	10.7212	7.2668	8.5874	2.5755	1.6877	3.0003
2A-3_87	0.0000	0.1783	3.7568	2.3126	1.4085	1.1806	10.2759	0.7804	8.7000	6.2165	7.6368	2.2284	1.4964	2.8138
1C-4_89	0.0385	0.1393	6.2070	2.9679	0.4778	0.3682	7.6478	0.4598	2.5036	2.0408	6.8577	0.6807	0.2643	0.4617
2B-2_87	0.0000	0.1791	3.6505	2.3256	1.4105	1.1738	10.2720	0.7759	8.4340	5.9987	7.4567	2.1653	1.4361	2.5803

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2A-7_87	0.0000	0.2303	4.8585	3.0099	1.8595	1.5612	8.2601	0.5677	8.5402	6.7607	8.1327	2.5193	1.7876	3.3788
3B-5_87	0.0000	0.2685	2.8740	1.6602	0.9795	0.8725	12.3594	0.8624	10.4138	7.1041	8.4154	2.4924	1.6051	2.9001
3C-17_87	0.0000	1.6448	13.2148	8.7467	5.3615	5.6108	0.0150	0.0000	0.0056	0.0153	0.0042	0.0509	0.2988	2.0721
3C-4_87	0.0000	0.2580	2.7606	1.6112	0.9372	0.8568	12.3212	0.8759	10.3980	6.8397	8.1566	2.4066	1.5646	2.8806
3B-14_89	0.0000	0.4272	6.0806	3.8317	2.2961	2.0391	0.4962	0.0000	3.5252	7.3840	3.7513	2.0037	1.7142	5.7570
2B-15_87	0.0000	0.7598	15.4070	10.7155	6.6462	5.8415	0.0000	0.0000	0.0945	1.0815	0.4996	1.0382	1.5191	4.6390
1B-6_87	0.0439	0.1438	6.5257	3.0358	0.4312	0.3319	9.7276	0.3714	3.6641	3.1762	0.7560	1.0118	0.4015	0.6176
3B-14_87	0.0000	0.7572	7.6187	4.4969	2.6455	2.7094	0.1837	0.0000	1.3040	4.3049	2.9091	2.3946	2.2843	4.8783
2A-5_87	0.0000	0.1711	4.4350	2.9061	1.7997	1.6086	9.1395	0.7517	7.8485	5.8530	7.6388	2.1715	1.5154	2.9337
4A-15_87	0.1242	0.1332	6.2165	3.3428	0.9046	0.6315	0.0856	0.0000	1.0921	3.8157	2.9223	2.8182	3.0297	6.3692
2A-18_87	0.0000	1.7247	26.1593	21.5663	14.7261	14.5669	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4677
1B-16_89	0.1362	0.6608	32.0030	17.6649	3.0952	2.6320	0.0000	0.0000	0.0000	0.0129	0.0765	0.0637	0.0297	0.3459
2C-11_89	0.0010	0.1503	2.6951	1.7270	1.0008	0.8802	6.0766	0.1436	11.0705	9.0485	6.4107	1.6562	1.2071	3.2243
4A-9_87	0.0307	0.0402	2.2156	1.1648	0.2991	0.2004	8.5193	0.6063	21.1249	7.0892	11.5284	3.0503	2.2106	3.4780
2A-11_89	0.0000	0.1760	3.0878	1.9805	1.1428	0.9723	6.8800	0.1605	12.7197	10.5514	7.2576	1.9582	1.4072	3.7782
1C-10_87	0.0530	0.2019	9.9061	4.6780	0.7254	0.5580	6.6615	0.2211	3.3862	3.6361	0.8207	1.2583	0.5312	0.8497
4B-13_87	0.0630	0.0721	3.6747	1.9379	0.5147	0.3551	2.1794	0.0432	9.1136	7.4004	9.1091	3.7143	3.0252	5.1696
3A-19_89	0.0000	1.9208	14.5146	12.6187	8.7964	9.2135	0.0056	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3912
4C-13_87	0.0580	0.0674	3.4872	1.8333	0.4585	0.3208	2.2320	0.0509	9.3654	7.2944	9.1253	3.5841	2.9485	4.9630

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
4A-12_87	0.0429	0.0532	2.7773	1.4500	0.3712	0.2534	5.4774	0.2505	15.5426	7.7169	11.2267	3.4853	2.6337	4.2250
2A-10_89	0.0000	0.1469	2.2135	1.3812	0.7844	0.6604	9.1981	0.2685	14.0889	10.1988	7.1041	1.8305	1.2497	3.2123
2B-8_87	0.0000	0.2390	5.4109	3.3922	2.0970	1.8299	8.0656	0.5384	8.6148	7.0458	8.4801	2.6182	1.8547	3.4344
2B-6_89	0.0000	0.1231	1.9110	1.1818	0.6756	0.5443	11.6650	0.4840	14.4628	9.5498	7.1717	1.6190	1.0751	2.7025
1B-15_89	0.1068	0.4560	25.7632	13.5207	2.3358	1.8932	0.0000	0.0000	0.0000	0.2713	0.8283	0.2171	0.1708	0.5681
1B-5_87	0.0512	0.1354	5.5562	2.5465	0.3990	0.2979	9.6898	0.3697	3.6470	3.0462	0.6987	0.9802	0.3823	0.6087
4C-5_87	0.0238	0.0277	1.7532	0.9064	0.2279	0.1503	10.0459	0.8639	20.0386	6.3821	10.8062	2.6623	1.8626	2.8334
2C-12_87	0.0000	0.3432	7.1340	4.5568	2.7482	2.3105	4.3236	0.1933	6.9202	7.2444	8.0055	2.8800	2.1493	4.1434
2C-16_89	0.0000	0.7104	9.2841	6.0501	3.5721	3.0841	0.0061	0.0000	0.0341	0.5923	0.0533	0.4317	0.7847	4.7936
2A-17_87	0.0000	1.1608	19.2623	13.5556	8.7511	7.8512	0.0000	0.0000	0.0000	0.0118	0.0000	0.0590	0.3903	2.4316
2A-16_87	0.0000	0.8442	16.8739	11.5262	7.2244	6.3425	0.0000	0.0000	0.0000	0.4720	0.1416	0.5842	1.0835	3.9251
2A-3_87	0.0000	0.1709	3.8826	2.4826	1.4261	1.2526	10.8874	0.8972	8.6502	6.1817	7.7385	2.2039	1.5052	2.7471
3A-12_89	0.0000	0.2270	3.2793	1.9854	1.1749	1.0615	6.2620	0.1476	12.1481	10.6303	8.3160	2.0778	1.4393	3.9783
1A-10_89	0.0546	0.2115	8.7163	4.2091	0.7110	0.5378	5.6403	0.3281	2.4359	2.4706	7.9195	0.8265	0.3370	0.6078
3C-12_89	0.0000	0.2025	3.0388	1.8742	1.1082	0.9553	6.1596	0.1722	11.2666	9.6280	7.7784	1.8560	1.2901	3.4813
2A-15_89	0.0000	0.4914	7.1575	4.6214	2.6265	2.2379	0.0357	0.0000	0.6330	3.3857	0.8709	1.3190	1.4848	6.0436
1B-14_87	0.1453	0.3608	12.6350	5.9642	0.9526	0.7121	0.2679	0.0000	0.5658	2.0578	0.3425	0.9948	0.5433	1.0144
3B-6_89	0.0000	0.1385	2.0259	1.2235	0.7182	0.6593	11.0816	0.5416	13.2878	9.0150	8.1997	1.5790	1.0433	2.6612
1B-1_87	0.0362	0.1342	6.1448	2.9753	0.4495	0.3503	8.5395	0.3123	2.9089	2.4878	0.5548	0.7373	0.2672	0.5189

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2B-4_87	0.0000	0.1890	4.0701	2.5441	1.5865	1.4162	11.3197	0.8754	9.1794	6.5887	8.1083	2.4198	1.6478	2.9450
4C-15_87	0.1101	0.1212	5.7119	3.0520	0.8203	0.5684	0.1533	0.0000	1.7052	4.4265	3.6976	3.0408	3.0923	6.2569
2C-7_87	0.0000	0.2349	3.9660	2.4327	1.4482	1.1806	9.3504	0.5851	9.1747	7.0427	8.1513	2.5263	1.7813	3.0487
1A-8_89	0.0370	0.1755	7.6596	3.7087	0.5683	0.4677	8.2574	0.5340	2.7972	2.3891	8.3565	0.7823	0.2966	0.5679
2C-11_89	0.0000	0.1523	2.5358	1.6046	0.9285	0.7844	6.4061	0.1536	11.4403	9.2230	6.3643	1.6744	1.2095	3.1772
2C-8_87	0.0000	0.2430	3.7218	2.2476	1.3245	1.0959	8.8618	0.5154	9.2535	7.0872	8.0241	2.5359	1.7641	3.0260
1A-19_87	0.3879	2.1864	40.2527	27.7939	5.0935	4.6551	0.0058	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0044
1A-16_87	0.1881	0.5467	19.4800	9.6866	1.5996	1.2319	0.0000	0.0000	0.0000	0.1719	0.0207	0.1817	0.1902	0.6081
3C-13_87	0.0000	0.5803	5.8458	3.4751	2.0476	2.0004	1.3572	0.0212	4.3561	6.8097	5.8729	3.0036	2.4108	4.7965
3C-8_89	0.0000	0.1519	2.3045	1.3875	0.8193	0.7420	9.9260	0.4389	13.0077	9.2440	8.2831	1.6698	1.1271	2.9132
3B-13_87	0.0000	0.6049	6.2423	3.7014	2.1782	2.1356	0.9796	0.0113	3.5571	6.4276	5.2771	2.9590	2.4410	4.9577
4A-18_87	0.4449	0.8661	18.8293	13.7195	3.9858	3.1821	0.0219	0.0000	0.0065	0.0000	0.0000	0.0000	0.0050	0.3993
2C-14_87	0.0000	0.5070	10.9007	7.0573	4.3635	3.6995	0.1707	0.0000	1.0819	3.5915	2.6972	2.0829	2.0355	4.8543
3A-18_87	0.0000	2.0430	13.4930	10.0059	6.3993	6.6324	0.0114	0.0000	0.0089	0.0000	0.0000	0.0000	0.0480	0.8714
2B-12_87	0.0000	0.3512	6.5965	4.1206	2.4930	2.0770	3.2483	0.1318	6.4316	7.2467	7.3966	2.9415	2.2145	4.2182
1C-17_87	0.2662	0.8539	26.3906	13.9331	2.3600	1.8576	0.0087	0.0000	0.0051	0.0000	0.0000	0.0205	0.0335	0.3103
2C-18_89	0.0000	1.9563	11.3932	10.7242	7.5462	8.2610	0.0068	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1511
3B-3_87	0.0000	0.2484	2.6247	1.5451	0.9027	0.8137	12.7350	0.9016	10.4337	6.7887	7.9928	2.3783	1.5628	2.7818
2B-16_87	0.0000	1.0678	17.0236	11.6263	7.4026	6.5218	0.0055	0.0000	0.0000	0.0908	0.0199	0.1762	0.5805	2.8724

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
3A-14_89	0.0000	0.4184	5.8893	3.8634	2.3061	2.0367	0.5434	0.0000	3.6432	7.4936	3.7894	2.0068	1.7711	5.7465
3A-14_87	0.0000	0.6324	6.4327	3.7735	2.2652	2.1863	0.4752	0.0000	2.2655	5.1366	3.9009	2.5281	2.2178	4.8126
2C-16_87	0.0000	0.8465	14.4060	9.4089	5.9073	5.1255	0.0000	0.0000	0.0407	0.7223	0.2406	0.7647	1.2401	4.1897
3B-7_89	0.0000	0.1514	2.3760	1.4546	0.8490	0.7774	10.8199	0.5193	13.8624	9.5947	8.5994	1.7124	1.1361	2.9266
3B-2_89	0.0000	0.1168	1.6633	0.9914	0.5834	0.4868	12.4454	0.6841	13.3343	8.3875	7.8158	1.4592	0.9465	2.3280
2A-11_87	0.0000	0.3036	5.5431	3.5151	2.1299	1.7785	5.2268	0.2501	7.6226	7.3220	8.0962	2.8082	2.1017	3.8805
1A-15_89	0.1119	0.3976	17.2491	8.5943	1.4825	1.1619	0.0491	0.0000	0.1515	0.8814	2.3750	0.4904	0.3247	0.7290
3A-17_89	0.0000	1.0122	9.4363	6.3890	3.8458	3.4609	0.0077	0.0000	0.0000	0.1266	0.0109	0.1571	0.4247	3.5959
3C-6_87	0.0000	0.2923	3.0485	1.7650	1.0519	0.9404	11.9856	0.8031	10.7497	7.4975	8.7232	2.6289	1.7453	3.1329
1C-6_89	0.0256	0.1503	7.2671	3.5560	0.5471	0.4380	8.9925	0.6241	2.7124	2.1987	7.9904	0.6841	0.2570	0.5074
3A-11_89	0.0000	0.1921	3.0262	1.8456	1.1069	0.9981	6.4304	0.1969	11.3353	9.5665	7.7951	1.8365	1.2708	3.4763
2A-9_89	0.0000	0.1337	2.1085	1.2776	0.7375	0.6510	9.9921	0.3481	12.9221	9.6404	7.0784	1.7091	1.1444	2.9361
2A-11_89	0.0000	0.1778	3.0777	1.9663	1.1344	0.9622	6.7760	0.1699	12.2283	10.5485	7.2432	2.0066	1.4167	3.7681
4B-9_87	0.0321	0.0384	2.1180	1.1014	0.2761	0.1830	8.6151	0.6157	20.4847	7.1143	11.6150	3.0492	2.1846	3.4430
1A-18_89	0.2086	0.7926	31.8445	17.3858	3.0901	2.5582	0.0000	0.0000	0.0000	0.0000	0.0121	0.0239	0.0235	0.2984
4A-17_87	0.2457	0.3135	11.1878	6.6275	1.7648	1.3108	0.0120	0.0000	0.0063	0.1139	0.0193	0.3236	0.9210	3.9569
2A-3_89	0.0000	0.0889	2.2152	1.4348	0.8077	0.7656	11.4106	0.7119	11.8091	7.8595	6.9136	1.3321	0.8672	2.2729
3C-14_89	0.0000	0.3782	5.6932	3.5836	2.1361	1.8784	0.8659	0.0000	4.6337	8.3015	4.6475	2.1024	1.7453	5.5384
2B-18_87	0.0000	2.0641	26.3488	22.6821	15.7904	17.2055	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1748

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
1B-13_87	0.1199	0.3058	12.0076	5.6206	0.9153	0.7016	1.0368	0.0138	1.3275	2.9132	0.5353	1.2324	0.6007	1.0186
2A-18_89	0.0000	1.4068	13.7752	10.8341	7.0300	7.1433	0.0000	0.0000	0.0080	0.0023	0.0000	0.0000	0.0049	0.7807
4C-17_87	0.2553	0.3343	11.7776	6.9195	1.9211	1.3593	0.0177	0.0000	0.0065	0.0815	0.0122	0.2656	0.8230	3.7795
2B-5_89	0.0000	0.1156	1.9241	1.2105	0.6987	0.6053	11.3108	0.5122	13.5150	8.7749	6.8835	1.5113	1.0035	2.5673
2A-9_89	0.0000	0.1399	2.0487	1.2350	0.7127	0.6282	10.1437	0.3370	13.9689	9.9039	7.0286	1.7057	1.1452	2.8957
4B-7_87	0.0327	0.0342	1.9703	1.0230	0.2547	0.1710	9.5032	0.7402	21.8151	6.8768	11.3753	2.9127	2.0731	3.2385
3B-4_89	0.0000	0.1362	1.7409	1.0284	0.5940	0.5207	12.8456	0.6623	14.3629	8.9898	7.9389	1.5634	1.0203	2.5093
2C-6_89	0.0000	0.1158	2.0114	1.2480	0.7181	0.5912	10.6779	0.4688	13.2284	8.6558	6.8593	1.5201	1.0154	2.5800
2C-8_89	0.0000	0.1154	1.8005	1.0826	0.6164	0.5048	9.7342	0.3699	12.9572	8.5929	6.4213	1.5002	1.0001	2.5141
3C-10_89	0.0000	0.1709	2.8295	1.7285	1.0360	0.9498	8.2921	0.3311	12.4794	9.5768	8.4085	1.7923	1.2145	3.2152
3A-1_89	0.0000	0.1132	1.4387	0.8431	0.4795	0.4225	11.0168	0.6044	12.0647	7.6603	6.9711	1.3464	0.8593	2.0983
1B-14_87	0.1149	0.3453	14.7239	7.0281	1.1409	0.8523	0.2537	0.0000	0.5414	1.9611	0.3498	0.9609	0.4940	0.9859
2B-1_87	0.0000	0.1388	2.6076	1.6315	1.0075	0.8516	10.3698	0.8106	7.6918	5.1427	6.3136	1.8648	1.2391	2.2212
3C-4_89	0.0000	0.1208	1.7441	1.0404	0.5950	0.5362	11.7011	0.6142	12.8942	8.3090	7.7396	1.4473	0.9331	2.3725
4B-10_87	0.0339	0.0447	2.3097	1.2098	0.3051	0.2010	7.4805	0.4728	19.1313	7.2761	11.4858	3.1731	2.3005	3.5639
2B-12_89	0.0000	0.1889	3.1426	1.9930	1.1429	0.9825	4.8413	0.0863	9.8707	9.7312	6.3850	1.8568	1.3904	3.7633
1B-10_89	0.0677	0.2255	9.5546	4.5648	0.7485	0.5895	5.2756	0.2929	2.4781	2.5868	8.2148	0.9503	0.4046	0.6825
3A-10_89	0.0000	0.1854	2.7563	1.6829	0.9800	0.8833	8.4977	0.2990	12.5749	10.1469	8.6669	1.8814	1.2557	3.3517
1C-8_87	0.0560	0.1737	8.4896	3.9692	0.6200	0.4710	8.0542	0.2927	3.6094	3.4707	0.7963	1.1608	0.4623	0.7559

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
3C-19_87	0.0000	3.8254	12.2494	12.5384	9.3063	11.1651	0.0168	0.0000	0.0056	0.0000	0.0000	0.0000	0.0000	0.0092
1C-6_87	0.0358	0.1469	6.4922	3.0065	0.4759	0.3366	10.1992	0.4098	3.8363	3.3258	0.7467	1.0736	0.3954	0.6589
2A-8_89	0.0000	0.1264	1.8787	1.1390	0.6552	0.5543	10.2149	0.3800	13.8246	9.4358	6.9109	1.6739	1.2149	2.8075
3C-12_89	0.0000	0.2079	3.0232	1.8661	1.1047	0.9891	6.2037	0.1687	11.2694	9.6513	7.7775	1.8570	1.3161	3.4820
3C-6_89	0.0000	0.1377	1.9733	1.1826	0.6917	0.5908	10.4365	0.5148	12.7076	8.5903	7.7954	1.5343	1.0205	2.5766
3A-17_89	0.0000	0.9940	10.8800	7.3350	4.4960	4.0239	0.0061	0.0000	0.0074	0.1328	0.0117	0.1611	0.4325	3.6863
1B-1_89	0.0315	0.1125	4.6108	2.1777	0.3506	0.2648	7.5692	0.4603	2.2616	1.7290	5.6808	0.5494	0.2160	0.3691
3A-19_89	0.0000	1.9509	12.6490	10.8911	7.4770	7.7736	0.0063	0.0000	0.0000	0.0000	0.0000	0.0024	0.0000	0.3743
1B-2_87	0.0561	0.1160	3.6011	1.5941	0.2548	0.1836	10.6751	0.4093	3.6099	2.7233	0.5862	0.8460	0.3354	0.4961
2C-12_87	0.0000	0.3318	7.3806	4.7043	2.9009	2.4653	4.4885	0.2245	6.9193	7.2293	7.9292	2.9156	2.1729	4.1768
3B-5_89	0.0000	0.1291	1.6849	0.9935	0.5747	0.5014	11.2384	0.5558	13.0073	8.3298	7.5708	1.4708	0.9726	2.3946
3C-18_89	0.0013	1.2080	12.0335	8.4715	5.2932	4.7620	0.0059	0.0000	0.0055	0.0117	0.0000	0.0294	0.1763	2.3909
3B-2_87	0.0000	0.2287	2.4452	1.4529	0.8157	0.7599	12.3433	0.9016	9.8798	6.3822	7.5941	2.2163	1.4736	2.6447
3B-11_89	0.0000	0.1977	3.1361	1.9121	1.1303	1.0351	7.2570	0.2253	12.6507	10.4041	8.5986	1.9726	1.3701	3.6580
3A-9_89	0.0000	0.1636	2.6598	1.6294	0.9415	0.8604	8.8360	0.3808	12.7479	9.5058	8.3088	1.7412	1.1435	3.0936
1B-6_89	0.0557	0.1709	6.4079	3.0007	0.5099	0.3874	8.1566	0.4576	2.8801	2.3627	7.7529	0.8141	0.3436	0.5422
3A-11_89	0.0000	0.1898	2.9705	1.8249	1.0816	0.9714	6.5415	0.1874	11.4951	9.6511	7.7768	1.8605	1.2704	3.4598
4C-18_87	0.3768	0.6001	16.7264	10.7573	3.1358	2.3273	0.0160	0.0000	0.0067	0.0000	0.0000	0.0074	0.1037	1.2496
3C-4_89	0.0000	0.1243	1.7464	1.0493	0.5985	0.5420	11.6850	0.6178	13.1989	8.4293	7.7301	1.4698	0.9593	2.4195

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
1A-7_87	0.0429	0.1584	7.3220	3.3833	0.5132	0.3966	9.1324	0.3639	3.8007	3.3871	0.7880	1.1433	0.4163	0.7212
4A-14_87	0.0831	0.0967	4.7047	2.5341	0.6374	0.4535	0.4770	0.0000	3.5012	5.5539	5.5191	3.3202	3.0603	5.7417
3C-16_89	0.0000	0.6661	8.1110	5.3495	3.1930	2.8526	0.0000	0.0000	0.3189	2.2143	0.5616	1.0241	1.2947	5.7961
4A-10_87	0.0375	0.0465	2.4166	1.2619	0.3191	0.2198	7.5899	0.4762	9.6539	7.5571	11.8739	3.2878	2.3972	3.7627
1C-2_87	0.0483	0.1105	3.4904	1.5548	0.2482	0.1749	10.0582	0.3865	3.4192	2.5661	0.5565	0.7973	0.2998	0.4553
1C-9_89	0.0528	0.1917	8.4388	4.0568	0.6904	0.5224	6.9629	0.3998	2.7099	2.5071	8.2680	0.8426	0.3559	0.6014
2B-17_87	0.0000	1.3472	23.8609	17.1032	11.2242	11.0818	0.0000	0.0000	0.0058	0.0000	0.0000	0.0104	0.1270	1.5631
1B-2_87	0.0527	0.1158	3.6027	1.6016	0.2574	0.1824	10.7596	0.4020	3.6268	2.7436	0.5858	0.8615	0.3394	0.4948
1A-15_87	0.1509	0.4258	15.9490	7.7439	1.2742	0.9706	0.0150	0.0000	0.0710	0.7570	0.1026	0.5199	0.3452	0.8317
1A-6_89	0.0553	0.1654	6.3777	3.0263	0.4859	0.3866	8.1163	0.4541	2.8188	2.2572	7.3362	0.7906	0.3191	0.5195
4C-16_87	0.1711	0.1986	8.2122	4.4723	1.2227	0.8322	0.0161	0.0000	0.1214	1.4831	0.6885	1.6202	2.3338	6.1044
3C-11_87	0.0000	0.3711	3.9514	2.2986	1.3720	1.2127	5.8346	0.2993	9.0355	7.9210	8.3532	2.9103	2.0556	3.7378
4C-1_87	0.0131	0.0217	1.4098	0.7272	0.1822	0.1208	10.0435	0.9317	8.6363	5.4650	9.5940	2.2565	1.5831	2.3514
1C-16_89	0.1531	0.6053	27.2279	14.4589	2.5417	2.0908	0.0000	0.0000	0.0000	0.0698	0.1662	0.0981	0.0930	0.4379
1A-7_87	0.0468	0.1618	7.7599	3.6278	0.5648	0.4191	8.7716	0.3546	3.6800	3.4382	0.7969	1.1252	0.4299	0.7327
2A-12_87	0.0000	0.3420	5.2197	3.1437	1.9042	1.5753	4.4761	0.1693	7.5956	7.5208	7.6789	2.9498	2.1502	4.0532
2B-7_89	0.0000	0.1312	2.1251	1.2757	0.7345	0.6475	11.5896	0.4596	14.7694	9.7591	7.4581	1.6864	1.1485	2.9201
4B-4_87	0.0224	0.0324	1.7114	0.8930	0.2266	0.1493	10.3990	0.9088	20.8807	6.3682	10.8807	2.6541	1.8645	2.8666
3B-8_89	0.0000	0.1518	2.3850	1.4422	0.8522	0.7538	10.3016	0.4617	13.1299	9.6457	8.5110	1.7289	1.1384	2.9563

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2A-15_89	0.0000	0.4873	6.9829	4.5003	2.5711	2.2333	0.0235	0.0000	0.6341	3.4353	0.8643	1.3163	1.4700	6.0226
1B-4_89	0.0358	0.1358	6.1562	2.9509	0.4768	0.3576	7.9161	0.4771	2.4368	2.0036	6.9630	0.6657	0.2474	0.4548
2A-2_89	0.0000	0.0866	1.8364	1.1984	0.6571	0.6174	12.0046	0.6987	12.6572	8.0208	6.6272	1.3862	0.9094	2.2342
1C-12_89	0.0669	0.2467	11.9378	5.8166	0.9941	0.7838	3.1182	0.1729	1.8874	2.4325	8.0030	0.9037	0.3830	0.6998
2A-14_89	0.0000	0.3955	6.7669	4.2811	2.4562	2.1560	0.2245	0.0000	2.0971	6.2025	2.2610	1.8110	1.7121	6.2034
1A-16_89	0.1591	0.5207	21.0615	10.6831	1.8490	1.4602	0.0000	0.0000	0.0082	0.2858	0.7198	0.2470	0.2110	0.6403
2B-18_87	0.0000	2.0774	23.6039	19.9932	13.8468	14.8939	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1954
1B-2_89	0.0412	0.1305	4.8452	2.2770	0.3639	0.2768	8.3197	0.4742	2.5554	1.9391	6.4128	0.6237	0.2498	0.4096
4B-15_87	0.2667	0.3676	12.1727	7.3285	2.0444	1.4906	0.0131	0.0000	0.0245	0.1305	0.0740	0.2224	0.6869	3.2738
3C-16_89	0.0000	0.6715	7.8009	5.1189	3.0400	2.7019	0.0074	0.0000	0.3057	2.2155	0.5686	1.0331	1.2920	5.7222
3C-15_89	0.0000	0.4761	6.7717	4.2883	2.5407	2.2738	0.2244	0.0000	2.0613	6.0818	2.6855	1.8398	1.6940	5.9744
4C-4_87	0.0238	0.0305	1.7053	0.8852	0.2279	0.1520	10.3967	0.8984	9.6564	6.3501	10.7450	2.6485	1.8775	2.7933
3A-1_89	0.0000	0.1120	1.4684	0.8673	0.4919	0.4387	11.1023	0.5934	12.1047	7.4979	6.9236	1.3168	0.8481	2.1069
1A-4_89	0.0378	0.1348	6.0814	2.9055	0.4606	0.3471	8.0279	0.4990	2.3825	1.9886	6.7575	0.6475	0.2386	0.4396
2A-19_87	0.0000	2.4717	26.6881	25.9633	18.9842	22.3254	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0242
1B-3_89	0.0366	0.1363	5.2025	2.4259	0.4017	0.3051	8.3419	0.4764	2.5914	2.0161	6.6899	0.6614	0.2528	0.4381
1A-6_89	0.0484	0.1648	6.6207	3.1399	0.5174	0.3997	8.0536	0.4621	2.7746	2.2893	7.5047	0.7687	0.3248	0.5203
1B-4_89	0.0478	0.1435	5.4712	2.5842	0.4207	0.3235	8.3447	0.4864	2.6424	2.0754	6.9097	0.6979	0.2829	0.4608
2B-16_87	0.0000	1.0477	17.6783	12.3492	7.8076	6.8906	0.0000	0.0000	0.0000	0.0811	0.0167	0.1582	0.5659	2.8798

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
4C-3_87	0.0247	0.0277	1.6459	0.8510	0.2135	0.1362	10.4824	0.9255	9.5371	6.2070	10.6226	2.5893	1.8174	2.6951
3B-13_89	0.0000	0.3094	4.5511	2.8534	1.7079	1.4928	1.9620	0.0138	6.8790	9.4490	6.0133	2.1021	1.6464	4.8905
1A-1_89	0.0326	0.1082	4.8430	2.3156	0.3551	0.2832	7.6259	0.4771	2.1989	1.7138	5.8911	0.5516	0.2144	0.3689
3A-17_87	0.0000	1.2580	11.3714	7.0746	4.2043	4.2207	0.0113	0.0000	0.0054	0.2793	0.0500	0.4022	0.8558	3.6260
1A-11_89	0.0697	0.2302	10.7549	5.2384	0.8833	0.6765	4.2790	0.2249	2.1475	2.4527	8.1149	0.8983	0.3688	0.6693
1A-2_89	0.0371	0.1237	4.6930	2.1877	0.3471	0.2615	8.6293	0.4821	2.4268	1.8842	6.3845	0.6136	0.2419	0.4027
3A-11_87	0.0000	0.3918	4.0575	2.4040	1.4143	1.2960	7.0300	0.3301	9.5262	8.2403	8.7103	3.0727	2.1322	4.0067
1B-17_89	0.2127	0.9099	36.2697	20.3869	3.6378	3.1120	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1866
1B-12_89	0.0876	0.2665	10.3724	4.9715	0.8349	0.6512	2.5653	0.1147	1.7866	2.4098	7.3224	0.9328	0.4231	0.7158
2B-14_89	0.0000	0.4104	6.5910	4.1853	2.4102	2.1088	0.2225	0.0000	2.0873	6.2051	2.3158	1.8146	1.6928	6.1453
3A-4_89	0.0000	0.1287	1.6063	0.9432	0.5400	0.4630	11.7580	0.5843	13.2545	8.3385	7.3776	1.4887	0.9640	2.3598
2B-3_89	0.0000	0.1029	1.7103	1.0417	0.5993	0.5265	12.6537	0.5824	14.1502	8.6694	6.7622	1.4750	0.9700	2.3996
2B-17_87	0.0000	1.3455	21.5603	15.3671	10.0578	10.0505	0.0000	0.0000	0.0000	0.0000	0.0000	0.0102	0.1456	1.5390
4A-15_87	0.1252	0.1347	6.1741	3.3262	0.8963	0.6281	0.0819	0.0000	1.0874	3.7905	2.9163	2.8098	3.0179	6.3408
3B-17_89	0.0000	1.2547	12.1270	8.7228	5.4789	4.9705	0.0057	0.0000	0.0000	0.0125	0.0000	0.0366	0.1941	2.5581
4A-16_87	0.1760	0.2042	8.4654	4.6440	1.2832	0.8826	0.0146	0.0000	0.0609	1.0361	0.4167	1.2833	2.0238	5.6749
1B-15_89	0.1163	0.4597	22.3840	11.6148	1.9825	1.6071	0.0000	0.0000	0.0000	0.3071	0.8184	0.2253	0.1626	0.6007
4B-4_87	0.0285	0.0316	1.7236	0.8890	0.2229	0.1527	10.4160	0.9114	20.4008	6.3988	10.8587	2.6761	1.8874	2.8238
2A-9_87	0.0000	0.2623	4.6403	2.8415	1.6840	1.3920	6.9277	0.4449	9.0509	7.3814	8.2680	2.7240	1.9647	3.4978

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
1C-15_87	0.1613	0.4397	17.0066	8.2528	1.3614	1.0512	0.0141	0.0000	0.0591	0.7128	0.1082	0.4991	0.3589	0.8650
1A-17_87	0.2239	0.7266	23.5427	12.1566	2.0530	1.6022	0.0000	0.0000	0.0000	0.0095	0.0000	0.0506	0.0640	0.4134
2C-16_89	0.0000	0.7049	9.4566	6.4665	3.8303	3.4552	0.0065	0.0000	0.0264	0.5845	0.0537	0.4320	0.7861	4.8916
3C-1_87	0.0000	0.1983	2.1120	1.2539	0.7045	0.6493	12.0398	0.8953	9.1393	5.8089	6.8488	1.9850	1.3100	2.2566
4A-2_87	0.0252	0.0296	1.5693	0.8074	0.2072	0.1429	10.2079	0.9124	19.4300	5.9532	10.0789	2.4549	1.7330	2.6439
4C-14_87	0.0838	0.0926	4.6490	2.4596	0.6602	0.4479	0.7346	0.0029	4.7059	6.1428	6.4320	3.4771	3.1128	5.7062
1B-14_89	0.0990	0.3701	16.4281	8.1725	1.3763	1.0940	0.0825	0.0000	0.2064	1.0404	2.9216	0.5362	0.3116	0.7310
1C-10_89	0.0624	0.2129	9.5559	4.6178	0.7734	0.5968	5.5858	0.3292	2.4577	2.4994	8.3050	0.8812	0.3658	0.6699
1A-5_89	0.0358	0.1437	6.4296	3.0796	0.5003	0.3739	7.9857	0.5029	2.4877	2.0649	7.0714	0.6851	0.2818	0.4639
1C-12_87	0.0968	0.2504	9.6751	4.4869	0.7093	0.5340	4.2267	0.1022	2.9394	3.7713	0.7592	1.3658	0.5985	0.9555
2A-18_89	0.0000	1.4123	13.6898	10.7073	6.9531	7.0262	0.0054	0.0000	0.0111	0.0000	0.0046	0.0000	0.0055	0.7853
1A-6_87	0.0283	0.1335	7.3291	3.4410	0.5264	0.3922	10.1116	0.4272	3.6862	3.1195	0.7326	1.0008	0.3291	0.6297
3A-15_87	0.0000	0.8066	7.9280	4.8188	2.8364	2.9188	0.0705	0.0000	0.7047	3.2020	1.8813	1.9421	2.0417	5.0369
3B-12_87	0.0000	0.4098	4.2585	2.5187	1.4426	1.3294	4.4363	0.1796	8.0670	7.8994	7.9241	3.0554	2.1657	4.0563
1A-19_87	0.3327	2.1128	45.0777	31.5056	5.9432	5.5054	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3A-18_87	0.0000	2.0370	14.7989	10.4055	6.6228	6.9562	0.0157	0.0000	0.0058	0.0000	0.0000	0.0000	0.0344	0.9085
3B-17_87	0.0000	1.8952	13.7600	9.6158	5.9512	6.0880	0.0114	0.0000	0.0074	0.0000	0.0000	0.0114	0.1231	1.2396
1A-1_87	0.0437	0.1033	3.2672	1.4510	0.2316	0.1637	10.1706	0.3980	3.3394	2.4588	0.5396	0.7695	0.3060	0.4456
3C-2_87	0.0000	0.2365	2.5181	1.4877	0.8767	0.7964	12.2371	0.8839	9.8345	6.3812	7.5976	2.2238	1.4634	2.6584

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2A-4_87	0.0000	0.1838	3.9084	2.5478	1.4926	1.3357	10.4247	0.8338	8.4483	6.1539	7.6884	2.2947	1.5003	2.8085
1C-4_87	0.0450	0.1300	5.2771	2.4100	0.3814	0.2852	9.6465	0.3792	3.5870	2.9184	0.6794	0.9541	0.3464	0.5589
3C-13_89	0.0000	0.3086	4.5141	2.7908	1.6433	1.4460	2.6523	0.0298	8.0769	10.1030	6.6606	2.1731	1.6388	4.7709
4B-1_87	0.0242	0.0243	1.4735	0.7614	0.1923	0.1288	10.0760	0.9383	18.6201	5.6178	9.7400	2.3183	1.6195	2.4826
3A-13_87	0.0000	0.5619	5.7086	3.3747	2.0194	1.9221	1.6635	0.0261	4.7230	7.0171	6.0726	3.0039	2.3849	4.7686
1B-11_89	0.0386	0.2353	12.5964	6.3871	0.9799	0.8225	3.9944	0.2572	1.9832	2.3009	8.5758	0.7355	0.3265	0.6645
1C-14_89	0.1035	0.3681	16.0784	7.9337	1.3726	1.0580	0.0661	0.0000	0.1816	0.9883	2.9225	0.5043	0.3028	0.7040
1C-5_89	0.0436	0.1462	6.4666	3.0981	0.5156	0.3932	7.9198	0.4808	2.5151	2.0871	7.0783	0.7103	0.2883	0.4773
4A-18_87	0.4364	0.8633	18.6930	13.6146	3.9587	3.1862	0.0162	0.0000	0.0073	0.0000	0.0000	0.0062	0.0068	0.3815
1B-10_89	0.0622	0.2186	9.8910	4.8143	0.7750	0.6056	5.4622	0.3315	2.4620	2.5414	8.6097	0.8660	0.3883	0.6655
3C-12_87	0.0000	0.3715	3.9799	2.3167	1.3744	1.2792	4.4172	0.1927	7.5998	7.2578	7.3479	2.7464	1.9773	3.7156
1B-3_89	0.0391	0.1334	5.3335	2.5165	0.4034	0.3102	8.1211	0.4788	2.5543	1.9679	6.5045	0.6555	0.2514	0.4355
2A-15_89	0.0000	0.4835	7.4109	4.8208	2.7749	2.4116	0.0403	0.0000	0.6448	3.3790	0.8699	1.3000	1.4805	6.0981
3C-18_89	0.0000	1.1990	12.4393	8.8174	5.5416	4.9977	0.0057	0.0033	0.0059	0.0107	0.0000	0.0310	0.1813	2.4357
2B-14_87	0.0000	0.5847	10.1277	6.4974	3.9556	3.3310	0.1173	0.0000	0.8608	3.3067	2.2024	1.9982	2.0918	4.9580
4A-7_87	0.0314	0.0335	1.9421	1.0165	0.2545	0.1713	9.3860	0.7390	9.8045	6.8398	11.3347	2.8994	2.0696	3.1826
3C-4_89	0.0000	0.1242	1.7004	1.0029	0.5716	0.4952	11.9601	0.6261	13.3465	8.3951	7.7662	1.4647	0.9573	2.3881
4A-3_87	0.0275	0.0308	1.6378	0.8459	0.2115	0.1420	10.1175	0.9001	19.1729	6.0949	10.4472	2.5513	1.8017	2.7356
2C-9_89	0.0000	0.1234	1.9396	1.2050	0.6886	0.5887	9.7686	0.3465	13.4584	9.2222	6.7898	1.6258	1.0847	2.7624

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
1C-14_87	0.1428	0.3809	14.9271	7.1617	1.1334	0.8740	0.0888	0.0000	0.2663	1.4745	0.2393	0.8283	0.4967	0.9897
3B-7_87	0.0000	0.3086	3.3121	1.9350	1.1237	1.0691	9.5950	0.6829	10.3428	7.6582	8.7989	2.7002	1.8318	3.1352
2B-11_89	0.0000	0.1688	2.9062	1.8473	1.0822	0.9577	6.2339	0.1406	11.7702	9.8848	6.7004	1.8286	1.3306	3.5900
1A-11_87	0.0550	0.2155	10.7699	5.1201	0.8324	0.6335	5.0892	0.1561	2.9513	3.5864	0.7908	1.2442	0.5381	0.9146
3C-9_89	0.0000	0.1598	2.3893	1.4646	0.8490	0.7603	9.5702	0.4050	13.0540	9.5062	8.4567	1.7450	1.1765	3.0404
2A-17_89	0.0000	0.9731	11.1762	7.5882	4.6131	4.1272	0.0065	0.0000	0.0000	0.0210	0.0000	0.0393	0.2184	2.7775
3C-14_89	0.0000	0.3797	5.7009	3.5490	2.1246	1.8650	0.8773	0.0000	4.6277	8.2464	4.6490	2.0774	1.7292	5.4681
2A-10_87	0.0000	0.2938	5.0576	3.1010	1.8495	1.5143	6.8103	0.3459	8.3984	7.4175	8.4266	2.7664	2.0087	3.5488
1C-1_89	0.0327	0.1075	4.5363	2.1378	0.3413	0.2657	7.6247	0.4464	2.2785	1.7187	5.6753	0.5727	0.2063	0.3725
4B-11_87	0.0400	0.0447	2.4698	1.2963	0.3269	0.2220	6.4667	0.3574	8.7117	7.3642	11.2645	3.2518	2.3987	3.8428
4B-2_87	0.0252	0.0272	1.6201	0.8367	0.2108	0.1353	10.3022	0.9169	20.4577	6.0665	10.3134	2.5191	1.7652	2.6369
1B-8_89	0.0486	0.1796	8.7688	4.2907	0.6744	0.5549	7.4711	0.4864	2.6726	2.3842	8.4196	0.7633	0.3050	0.5864
1A-5_87	0.0477	0.1394	5.8784	2.6916	0.4343	0.3184	9.3095	0.3501	3.5621	3.1077	0.6987	0.9993	0.4203	0.6095
2B-10_89	0.0000	0.1531	2.3420	1.4720	0.8339	0.7067	8.2807	0.2325	13.3358	10.1156	6.9231	1.7953	1.2490	3.2117
1A-8_87	0.0353	0.1652	8.5886	4.0234	0.6395	0.4687	8.1551	0.3266	3.4967	3.3984	0.8054	1.1333	0.4403	0.7600
3B-18_87	0.0000	3.0097	13.8312	12.0265	8.2461	9.1909	0.0136	0.0000	0.0079	0.0000	0.0000	0.0000	0.0000	0.0581
2B-7_87	0.0000	0.2514	4.0721	2.5583	1.5405	1.2609	8.7786	0.5369	8.9758	7.0707	8.1468	2.5669	1.7818	3.1603
3C-1_89	0.0000	0.1161	1.4865	0.8709	0.4957	0.4293	11.9999	0.6539	12.9758	7.9114	7.3639	1.3713	0.8911	2.1871
1C-6_89	0.0218	0.1441	7.9914	3.9649	0.5852	0.5276	8.8930	0.6611	2.6031	2.1134	8.0056	0.6442	0.2328	0.4860

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
3C-8_87	0.0000	0.3174	3.3005	1.9309	1.1334	1.1382	10.2191	0.6056	10.0283	7.4163	8.3244	2.6535	1.7958	3.1958
2B-11_87	0.0000	0.3367	5.8539	3.6288	2.1703	1.7869	3.8824	0.1656	7.0120	7.1591	7.7117	2.8768	2.0991	3.9343
1A-14_89	0.0756	0.3296	17.6856	9.0077	1.4871	1.2218	0.1951	0.0000	0.3247	1.2483	4.1220	0.5843	0.2605	0.7022
3A-13_89	0.0000	0.3254	4.6998	2.9708	1.7727	1.5317	2.0243	0.0143	6.9822	9.5474	6.1156	2.1499	1.6690	4.9580
2C-3_89	0.0000	0.0933	2.0316	1.3307	0.7141	0.6371	12.0365	0.7204	12.9553	8.3363	7.1526	1.4015	0.9062	2.3312
4B-10_87	0.0358	0.0423	2.3133	1.2025	0.3137	0.2163	7.4639	0.4724	9.2263	7.2995	11.4673	3.1744	2.2672	3.5624
4B-11_87	0.0350	0.0469	2.4561	1.2931	0.3293	0.2258	6.5124	0.3609	8.7896	7.4464	11.2578	3.2749	2.4145	3.8623
1A-3_87	0.0596	0.1315	4.0719	1.8142	0.2689	0.2054	11.3337	0.4292	3.9010	3.0303	0.6487	0.9449	0.3846	0.5503
4C-18_87	0.3713	0.5921	16.5063	10.6217	3.0832	2.2870	0.0151	0.0000	0.0000	0.0000	0.0000	0.0074	0.0980	1.2650
3A-16_89	0.0000	0.7343	9.3548	6.3565	3.8436	3.4547	0.0060	0.0000	0.1075	1.1610	0.1971	0.6913	1.0539	5.4720
4B-5_87	0.0258	0.0308	1.7442	0.9105	0.2273	0.1505	10.0972	0.8707	20.5601	6.3775	10.8769	2.6634	1.9029	2.8281
3A-7_89	0.0000	0.1536	2.2948	1.3839	0.8067	0.7202	10.8819	0.5036	13.9350	9.5913	8.6760	1.7262	1.1367	2.8920
1C-15_87	0.1599	0.4400	17.0258	8.2629	1.3640	1.0358	0.0095	0.0000	0.0515	0.7062	0.1087	0.5092	0.3548	0.8553
1B-12_87	0.0921	0.2397	9.2926	4.3261	0.6764	0.5123	4.7297	0.1194	3.1261	3.8184	0.7768	1.3691	0.6038	0.9409
2A-15_87	0.0000	0.6258	11.1688	7.4198	4.5422	3.9030	0.0539	0.0000	0.4732	2.5725	1.5652	1.7413	1.9382	4.9160
2C-10_89	0.0000	0.1498	2.4533	1.5444	0.8808	0.7314	8.6961	0.2629	13.4485	10.0325	7.2184	1.8358	1.2565	3.2445
3C-12_87	0.0000	0.3765	3.9411	2.3239	1.3729	1.2737	4.4320	0.1930	7.6454	7.2746	7.3733	2.7461	1.9676	3.6307
3A-12_87	0.0000	0.4072	4.2126	2.4976	1.4801	1.3277	5.0222	0.2300	8.5093	7.9776	8.2237	2.9896	2.1472	3.9796
2A-2_87	0.0000	0.1903	3.7445	2.3893	1.3640	1.1727	10.7318	0.8496	8.7126	6.2267	7.7634	2.2244	1.5217	2.6821

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2B-7_89	0.0000	0.1394	1.8413	1.0840	0.6071	0.5004	11.8892	0.4593	15.2032	10.1533	7.3595	1.6804	1.1291	2.7274
1C-9_87	0.0528	0.1749	8.2095	3.8236	0.5979	0.4662	7.9152	0.2759	3.6675	3.5832	0.7912	1.2088	0.5066	0.7907
2A-8_89	0.0000	0.1282	1.9038	1.1397	0.6556	0.5680	10.6579	0.3945	14.1543	9.4037	6.9812	1.6391	1.0929	2.7319
1A-7_89	0.0452	0.1648	6.7669	3.2363	0.5127	0.4025	8.2440	0.5062	2.7406	2.3199	7.6394	0.7545	0.2824	0.5237
3C-9_89	0.0000	0.1612	2.4977	1.5109	0.8831	0.7926	9.3589	0.3940	12.9157	9.4827	8.4452	1.7391	1.1451	3.0606
3A-1_87	0.0000	0.1967	2.1135	1.2637	0.6965	0.6576	12.1179	0.9074	9.1819	5.7429	6.8529	1.9793	1.3164	2.3315
1A-1_89	0.0314	0.1107	4.5609	2.1374	0.3394	0.2552	7.7175	0.4693	2.2187	1.7397	5.9085	0.5498	0.2084	0.3652
2C-16_87	0.0000	0.8519	14.1116	9.1665	5.7422	5.1308	0.0053	0.0000	0.0491	0.7237	0.2338	0.7736	1.2840	4.1843
2C-8_87	0.0000	0.2406	3.8382	2.3221	1.3932	1.1309	7.6171	0.5065	9.1760	7.0915	7.9734	2.6078	1.7803	3.0864
3B-12_87	0.0000	0.4157	4.2396	2.5181	1.4383	1.3369	4.8025	0.1778	8.0395	7.8523	7.9067	3.0351	2.1763	3.9683
1B-6_87	0.0441	0.1456	6.2815	2.9056	0.4289	0.3303	9.4192	0.3683	3.7111	3.1692	0.7296	1.0357	0.3474	0.6520
4B-6_87	0.0276	0.0317	1.8514	0.9603	0.2410	0.1573	9.9253	0.8207	21.3093	6.7175	11.3314	2.8281	2.0107	3.0569
2B-16_89	0.0000	0.8194	10.7703	7.2473	4.3302	3.8234	0.0000	0.0000	0.0000	0.1900	0.0147	0.1998	0.5091	4.0502
1B-8_89	0.0484	0.1909	9.2278	4.5140	0.7589	0.5630	6.8294	0.4542	2.4740	2.3197	8.2090	0.8088	0.3116	0.5732
3C-4_87	0.0000	0.2596	2.7555	1.5960	0.9478	0.8357	12.3222	0.8738	10.4102	6.8652	8.1520	2.3983	1.5756	2.8223
3B-5_89	0.0000	0.1289	1.7440	1.0337	0.5955	0.5244	10.9772	0.5471	12.8435	8.3347	7.6573	1.4597	0.9590	2.3855
2C-18_87	0.0000	1.8301	27.6844	22.3288	15.2297	16.5595	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3843
4C-4_87	0.0283	0.0311	1.7067	0.8826	0.2199	0.1504	10.3661	0.8966	9.5868	6.3443	10.7769	2.6371	1.8339	2.7995
1B-13_87	0.1282	0.3148	11.8452	5.5524	0.8783	0.6631	1.0798	0.0135	1.3339	2.8771	0.5338	1.2025	0.5959	1.0241

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
3C-19_87	0.0000	3.8261	12.2311	12.5499	9.2377	11.1491	0.0135	0.0000	0.0072	0.0000	0.0000	0.0000	0.0000	0.0046
2B-6_87	0.0000	0.2133	4.4424	2.7449	1.7006	1.3854	9.6319	0.6990	8.9970	6.8301	8.2224	2.4532	1.6750	3.2511
2A-12_89	0.0000	0.1910	3.1773	1.9880	1.1561	1.0508	5.8597	0.1074	12.0548	10.7191	7.0283	2.0652	1.4975	4.0225
2C-10_87	0.0000	0.2719	5.4644	3.4011	2.0864	1.8284	6.4262	0.3709	8.1280	7.2198	8.2072	2.7181	1.9583	3.7210
4B-16_87	0.3528	0.5763	15.3063	9.9648	2.7883	2.1532	0.0155	0.0000	0.0107	0.0293	0.0204	0.0447	0.2128	1.5117
4C-14_87	0.0898	0.0934	4.6503	2.4585	0.6591	0.4464	0.7596	0.0060	4.7312	6.2107	6.4268	3.5280	3.1554	5.7887
3B-10_89	0.0000	0.1764	2.8487	1.7570	1.0211	0.9268	8.1735	0.3059	12.6439	9.7650	8.3689	1.8388	1.2317	3.2977
1A-7_89	0.0309	0.1587	8.4077	4.1708	0.6441	0.5254	7.8712	0.5262	2.5705	2.1840	8.0104	0.6813	0.2499	0.5325
3C-10_87	0.0000	0.3350	3.5812	2.0802	1.2313	1.1590	7.9151	0.4284	9.4966	7.6415	8.3778	2.7634	1.8829	3.5002
2B-13_87	0.0000	0.4391	10.2335	6.6232	4.0951	3.5545	0.5676	0.0000	2.3503	4.9850	4.3682	2.4793	2.1993	4.7692
1A-12_87	0.0783	0.2400	10.9687	5.1566	0.8235	0.6499	3.7367	0.0934	2.6064	3.5876	0.7389	1.3130	0.5898	0.9687
1C-12_87	0.0943	0.2456	10.0024	4.6621	0.7431	0.5450	4.2790	0.1082	2.9534	3.7843	0.7805	1.3701	0.6033	0.9488
2C-16_89	0.0000	0.7084	9.4930	6.4945	3.8359	3.4741	0.0063	0.0000	0.0291	0.5791	0.0484	0.4295	0.7734	4.8375
2B-19_87	0.0000	3.0981	19.0991	22.2960	17.0034	21.4722	0.0000	0.0000	0.0098	0.0000	0.0000	0.0000	0.0000	0.0000
2A-6_89	0.0000	0.1220	2.1329	1.3449	0.7717	0.6344	11.5103	0.5032	14.3937	9.4966	7.4810	1.6668	1.1194	2.8110
1C-6_87	0.0446	0.1445	6.9513	3.2380	0.4928	0.3767	9.5616	0.4045	3.6324	3.1156	0.7563	1.0152	0.3750	0.6267
1B-14_89	0.0987	0.3717	16.4383	8.1968	1.3806	1.0855	0.0950	0.0000	0.2170	1.0340	3.0456	0.5330	0.3231	0.7211
1C-16_87	0.1903	0.5768	22.1751	11.2281	1.8502	1.4624	0.0000	0.0000	0.0000	0.1004	0.0082	0.1408	0.1610	0.5933
1A-17_89	0.1886	0.6255	23.8812	12.2675	2.1369	1.6954	0.0000	0.0000	0.0053	0.0684	0.1352	0.0979	0.1150	0.4831

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
1B-18_89	0.3983	5.7563	36.8047	42.7021	9.7532	12.5354	0.0040	0.0000	0.0053	0.0000	0.0000	0.0000	0.0000	0.0284
3A-15_89	0.0000	0.5212	7.8521	5.0673	3.0192	2.7201	0.0994	0.0000	1.1934	4.7803	1.8792	1.6310	1.6752	6.1576
1A-10_89	0.0561	0.2042	9.0152	4.3785	0.7040	0.5673	5.7362	0.3209	2.4177	2.4187	8.0086	0.8528	0.3436	0.6173
2A-17_89	0.0000	0.9549	12.7403	8.9574	5.4205	4.8956	0.0000	0.0000	0.0000	0.0163	0.0000	0.0359	0.2180	2.8308
2C-4_89	0.0000	0.0994	1.6470	1.0272	0.5920	0.5073	11.2499	0.5155	12.8155	8.1008	6.3803	1.3912	0.9150	2.3190
2C-2_87	0.0000	0.1639	3.3678	2.1906	1.2952	1.1971	12.3953	1.0651	8.3953	5.8048	7.7358	2.1523	1.3783	2.4556
1B-7_89	0.0575	0.1785	6.9036	3.2553	0.5497	0.4160	8.1088	0.4408	2.9045	2.4687	7.8458	0.8400	0.3556	0.5566
3B-3_89	0.0000	0.1244	1.7755	1.0484	0.6089	0.5421	11.6443	0.6178	13.1509	8.3067	7.8196	1.5862	1.2471	2.5158
2B-15_87	0.0000	0.7714	15.1271	10.3092	6.3618	5.5614	0.0000	0.0000	0.1063	1.1203	0.4900	1.0445	1.4984	4.6200
2A-2_89	0.0000	0.0960	1.7248	1.0479	0.6189	0.5277	12.2438	0.5911	13.4725	8.3654	6.6112	1.4348	0.9247	2.4034
1C-6_89	0.0364	0.1538	8.3707	4.1344	0.6825	0.5164	7.5425	0.5424	2.4136	2.1161	7.9161	0.6939	0.2579	0.5093
3B-2_89	0.0000	0.1204	1.7396	1.0399	0.6035	0.5268	12.3667	0.6822	13.1523	8.3715	7.8513	1.4515	0.9094	2.3199
2C-18_89	0.0000	1.9499	11.7606	11.1326	7.8225	8.6037	0.0059	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1553
4B-11_87	0.0366	0.0436	2.4766	1.3001	0.3244	0.2225	6.3951	0.3617	8.7533	7.3596	11.3006	3.2541	2.3888	3.8381
2A-3_89	0.0000	0.0966	1.7707	1.1021	0.6135	0.5435	11.2451	0.5583	12.1677	8.0656	6.5758	1.3884	0.9012	2.3031
4C-9_87	0.0305	0.0366	2.2223	1.1381	0.2822	0.1868	9.0898	0.6550	21.8971	7.5284	12.3200	3.2257	2.3290	3.5964
2C-3_87	0.0000	0.1838	4.1873	2.7491	1.6056	1.4553	11.8135	1.0443	8.8334	6.1769	8.2279	2.2565	1.5337	2.7670
1C-16_89	0.1320	0.5868	27.4862	14.7725	2.5638	2.1825	0.0000	0.0000	0.0000	0.0547	0.1677	0.0988	0.0597	0.4541
2A-14_87	0.0000	0.5292	10.6034	6.9382	4.2346	3.5052	0.3265	0.0000	1.7398	4.6521	3.6305	2.4512	2.3348	5.1457

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
3A-4_87	0.0000	0.2495	2.6491	1.5539	0.9132	0.8125	12.4704	0.8887	10.3038	6.7819	8.0398	2.3806	1.5709	2.8015
2C-6_87	0.0000	0.2073	4.5699	2.8563	1.7507	1.4592	9.6423	0.7292	8.7632	6.7022	8.1015	2.4397	1.6392	3.1340
4A-16_87	0.1646	0.2087	8.4830	4.6789	1.2352	0.8844	0.0103	0.0000	0.0629	1.0371	0.4136	1.2797	2.0428	5.7309
2A-16_89	0.0000	0.6644	10.6813	7.3865	4.3019	3.8727	0.0000	0.0000	0.0000	0.5696	0.0498	0.4159	0.7555	5.1843
2A-12_89	0.0000	0.1926	3.2566	2.0466	1.2103	1.0672	5.6697	0.1079	11.6496	10.7254	7.0763	2.0676	1.4984	4.0484
2A-13_89	0.0000	0.2626	5.7041	3.7163	2.1581	1.9497	1.4544	0.0000	5.9248	9.1172	5.0004	2.1141	1.6799	5.3828
1A-4_89	0.0424	0.1397	5.4961	2.5944	0.4061	0.3219	7.9807	0.4652	2.5405	1.9966	6.5780	0.6933	0.2581	0.4452
2C-3_89	0.0000	0.0907	2.0299	1.2900	0.7057	0.6503	11.9841	0.6730	12.9973	8.3114	6.7697	1.3940	0.9282	2.3705
2B-4_89	0.0000	0.1013	1.7636	1.1067	0.6238	0.5491	11.0834	0.5216	12.2749	8.2478	6.5983	1.4176	0.9246	2.4299
1B-18_87	0.2540	0.8357	27.6548	14.7276	2.4825	1.9927	0.0059	0.0000	0.0000	0.0000	0.0000	0.0213	0.0308	0.3294
1A-8_87	0.0581	0.1729	7.3260	3.3923	0.5330	0.4004	8.4852	0.2910	3.7812	3.5700	0.7828	1.2030	0.4950	0.7642
1B-16_87	0.1457	0.4622	19.7735	9.7902	1.6216	1.2586	0.0000	0.0000	0.0066	0.3709	0.0492	0.3039	0.2554	0.7501
1B-7_87	0.0430	0.1523	7.4408	3.4835	0.5468	0.4052	8.9638	0.3546	3.6170	3.2849	0.7727	1.0750	0.3849	0.6691
2A-8_87	0.0000	0.2446	4.4933	2.7846	1.6718	1.3753	8.6365	0.5576	9.0509	7.1194	8.2037	2.6257	1.8685	3.2901
2A-13_87	0.0000	0.4187	9.2748	5.9641	3.6864	3.0879	1.1595	0.0214	3.7005	6.0097	5.7323	2.7563	2.2440	4.7380
2B-4_89	0.0000	0.0950	1.8578	1.2076	0.6917	0.5835	11.1984	0.6050	12.5614	8.0827	6.4716	1.3575	0.9109	2.3415
2C-6_89	0.0000	0.1127	1.9590	1.2075	0.7093	0.5963	10.8907	0.4745	13.2648	8.7036	6.8051	1.4905	1.0059	2.5685
4C-13_87	0.0562	0.0658	3.4965	1.8436	0.4684	0.3398	2.3046	0.0487	9.2859	7.2763	9.1519	3.6236	2.9386	4.9455
2A-12_87	0.0000	0.3130	6.8007	4.3017	2.6334	2.1864	3.9038	0.2068	6.7802	7.1558	7.7957	2.8470	2.1662	4.2527

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
3B-10_87	0.0000	0.3525	3.7032	2.1839	1.2892	1.1737	7.9759	0.4240	9.7673	7.9247	8.6601	2.9112	1.9948	3.6927
4A-7_87	0.0327	0.0363	1.9203	1.0017	0.2555	0.1728	9.3911	0.7308	19.7110	6.8125	11.2302	2.8862	2.0750	3.1097
3B-18_87	0.0000	3.0100	13.7919	11.9568	8.2421	9.1637	0.0117	0.0000	0.0075	0.0000	0.0000	0.0000	0.0000	0.0552
3A-19_87	0.0000	2.5869	14.8357	11.5262	7.6633	8.2718	0.0152	0.0000	0.0051	0.0000	0.0000	0.0000	0.0000	0.2353
2C-3_87	0.0000	0.1877	4.1777	2.7240	1.5667	1.4278	11.1769	0.9691	8.7801	6.1688	8.1612	2.2405	1.4905	2.8098
1C-13_87	0.0938	0.3111	13.5936	6.5186	1.0372	0.7835	0.5624	0.0000	0.8558	2.4337	0.4457	1.0769	0.5448	0.9930
4A-4_87	0.0249	0.0298	1.7042	0.8907	0.2220	0.1531	10.3341	0.9091	19.9171	6.3985	10.8697	2.6525	1.8721	2.8590
4A-12_87	0.0417	0.0546	2.7645	1.4542	0.3672	0.2556	5.4798	0.2517	15.2942	7.6908	11.1846	3.4756	2.6057	4.1561
3A-4_89	0.0000	0.1263	1.7255	1.0221	0.6014	0.5273	11.5097	0.5896	13.0446	8.3382	7.6905	1.4595	0.9675	2.3710
3A-18_89	0.0000	1.3539	12.3972	9.1088	5.7868	5.2914	0.0061	0.0000	0.0000	0.0024	0.0000	0.0092	0.0778	1.6479
2C-7_89	0.0000	0.1140	1.6582	1.0188	0.5753	0.4867	10.8433	0.4261	13.4662	8.9307	6.5596	1.5079	1.0056	2.4866
3B-15_87	0.0000	0.9263	8.9586	5.4174	3.1740	3.2972	0.0291	0.0000	0.2815	2.1206	1.0413	1.5341	1.8418	4.7800
3A-7_87	0.0000	0.3061	3.2472	1.8877	1.1177	1.0481	11.4877	0.7597	10.6746	7.5824	8.8503	2.7186	1.7768	3.2136
1C-16_87	0.1912	0.5860	22.1892	11.2577	1.8280	1.4824	0.0000	0.0000	0.0000	0.1000	0.0124	0.1415	0.1342	0.6049
3A-2_87	0.0000	0.2354	2.5221	1.5079	0.8298	0.8159	12.6343	0.9368	9.9782	6.5100	7.8472	2.2986	1.5184	2.6674
1B-17_87	0.1935	0.6047	23.5445	12.0434	1.9925	1.5729	0.0000	0.0000	0.0000	0.0750	0.0061	0.1198	0.1245	0.5707
3A-19_87	0.0000	2.5871	14.6357	11.3782	7.5355	8.1923	0.0113	0.0000	0.0077	0.0000	0.0000	0.0000	0.0000	0.2491
1B-9_87	0.0668	0.1794	7.5431	3.4772	0.5555	0.4184	8.0835	0.2728	3.7795	3.6171	0.7842	1.2112	0.5046	0.7843
1C-17_89	0.2190	0.9119	32.4358	18.1291	3.2398	2.7342	0.0000	0.0000	0.0000	0.0000	0.0000	0.0053	0.0000	0.1851

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2A-17_89	0.0000	0.9699	11.2505	7.6450	4.6505	4.1311	0.0068	0.0000	0.0060	0.0227	0.0000	0.0398	0.2164	2.8011
2A-2_87	0.0000	0.1921	3.5127	2.1844	1.3177	1.0667	10.6130	0.7701	8.9543	6.2796	7.6235	2.2560	1.5107	2.7910
2A-16_87	0.0000	0.8536	14.7792	9.9382	6.1758	5.3819	0.0000	0.0000	0.0134	0.4957	0.1395	0.5952	1.0847	3.9083
4A-11_87	0.0406	0.0490	2.6104	1.3757	0.3553	0.2374	6.2981	0.3483	16.4752	7.5636	11.5435	3.3734	2.5005	3.9988
3A-11_89	0.0000	0.1973	2.8357	1.7147	1.0061	0.8744	6.6001	0.1939	11.6334	9.6377	7.9462	1.8675	1.2550	3.4388
1C-1_87	0.0447	0.1042	3.1705	1.4167	0.2128	0.1578	9.8115	0.3766	3.2448	2.4360	0.5185	0.7586	0.2945	0.4396
1C-5_87	0.0474	0.1379	5.4498	2.4905	0.3856	0.2931	9.5304	0.3738	3.5956	3.0381	0.6919	0.9669	0.3709	0.5794
2C-14_89	0.0000	0.3625	5.9277	3.7339	2.1385	1.8920	0.4162	0.0000	3.0002	7.1339	2.8925	1.8792	1.7208	5.8449
3A-3_87	0.0000	0.2466	2.6601	1.5432	0.9052	0.8163	12.7400	0.9252	10.4262	6.7053	8.0440	2.3506	1.5347	2.7576
3B-16_87	0.0000	1.2736	11.2482	7.1885	4.2521	4.2328	0.0156	0.0000	0.0057	0.2699	0.0553	0.3934	0.8266	3.6238
3A-8_89	0.0000	0.1430	2.1368	1.2922	0.7602	0.6748	8.7251	0.3786	11.7976	8.4992	7.6362	1.5574	1.0408	2.7182
2A-4_89	0.0000	0.1019	2.1544	1.3363	0.7797	0.6711	11.3940	0.5962	13.3413	8.7023	6.9927	1.5036	0.9848	2.5434
1A-9_89	0.0600	0.1983	7.8926	3.7719	0.6432	0.4982	6.8961	0.3943	2.7511	2.5543	8.0750	0.8958	0.3514	0.6121
1B-3_87	0.0632	0.1257	3.9220	1.7429	0.2764	0.1981	11.0268	0.4172	3.8232	2.9060	0.6217	0.9121	0.3590	0.5283
2C-14_89	0.0000	0.3675	5.7482	3.6103	2.0513	1.7906	0.4368	0.0000	3.0605	7.3104	2.9471	1.9170	1.9046	5.9817
1A-12_89	0.0938	0.2597	9.5570	4.5612	0.7651	0.5874	3.6019	0.1571	2.2580	2.6427	7.7165	0.9822	0.4552	0.7265
2C-15_87	0.0000	0.6493	12.2014	7.8641	4.9269	4.2124	0.0403	0.0000	0.3799	2.2332	1.2799	1.5975	1.8790	4.8859
2A-17_87	0.0000	1.1756	17.1655	11.7957	7.5389	7.3532	0.0096	0.0000	0.0000	0.0277	0.0000	0.0742	0.4054	2.3802
1C-5_89	0.0529	0.1537	5.2839	2.4623	0.4034	0.3048	9.1661	0.4929	2.8961	2.2380	7.1742	0.7438	0.3002	0.4856

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2C-5_89	0.0000	0.1112	1.9098	1.1865	0.6823	0.5595	12.1327	0.5490	15.1154	9.0339	7.1293	1.5747	1.0326	2.6113
4C-16_87	0.1574	0.1948	8.2516	4.4935	1.2174	0.8568	0.0116	0.0000	0.1159	1.4786	0.6847	1.6189	2.3498	6.1449
1A-17_89	0.1831	0.6128	23.8741	12.3907	2.1640	1.7591	0.0000	0.0000	0.0000	0.0678	0.1405	0.0926	0.1035	0.4563
3A-4_87	0.0000	0.2529	2.6936	1.5609	0.9142	0.8262	12.4417	0.8872	10.1690	6.7606	8.0655	2.3813	1.5764	2.7779
3B-5_87	0.0000	0.2657	2.8572	1.6898	0.9555	0.8660	12.3475	0.8569	10.4518	7.1410	8.3691	2.5188	1.6187	2.9385
3B-8_87	0.0000	0.3293	3.5150	2.0450	1.1957	1.0942	10.3711	0.6430	10.5098	7.8277	8.9891	2.7994	1.8553	3.3859
3B-3_87	0.0000	0.2534	2.6823	1.5751	0.8893	0.8179	12.5333	0.9066	10.3373	6.7339	8.0207	2.3527	1.5437	2.8017
1A-13_89	0.0770	0.2988	15.3856	7.7180	1.2779	1.0385	0.6735	0.0232	0.7247	1.6880	5.7384	0.6604	0.3310	0.7545
3B-4_89	0.0000	0.1334	1.8405	1.0982	0.6329	0.5451	12.4459	0.6578	14.1464	8.8911	8.3283	1.5447	1.0315	2.5115
3A-1_87	0.0000	0.1973	2.1225	1.2548	0.7041	0.6502	12.0855	0.9016	9.1822	5.7704	6.8675	2.0043	1.2870	2.2959
1B-12_89	0.0968	0.2698	9.2766	4.3859	0.7548	0.5681	2.6975	0.1117	1.8983	2.5228	7.2340	0.9584	0.4419	0.7257
1B-16_89	0.1803	0.6872	26.1114	13.8210	2.4300	1.9753	0.0000	0.0000	0.0067	0.0282	0.0719	0.0613	0.0571	0.3971
1C-12_87	0.0682	0.2289	11.8585	5.6440	0.8655	0.6724	4.3179	0.1235	2.7459	3.5959	0.7884	1.2646	0.5389	0.9442
3A-2_87	0.0000	0.2351	2.5389	1.5023	0.8514	0.7773	12.7304	0.9433	10.1802	6.6108	7.8552	2.2745	1.5304	2.7038
1C-13_89	0.1029	0.3477	13.8413	6.7807	1.1567	0.9079	0.5410	0.0139	0.7287	1.8341	5.1222	0.8222	0.4287	0.7844
1B-5_89	0.0428	0.1548	6.4929	3.1064	0.4994	0.3828	8.2652	0.4947	2.6861	2.1571	7.2642	0.7383	0.2928	0.4819
1B-5_89	0.0449	0.1549	6.2272	2.9704	0.4817	0.3855	8.1512	0.4849	2.6856	2.1614	7.1171	0.7125	0.3140	0.4896
2B-18_87	0.0000	2.0334	29.1024	26.0069	18.3808	19.9375	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1780
4C-1_87	0.0182	0.0263	1.3977	0.7185	0.1796	0.1241	9.8440	0.9272	17.6762	5.4119	9.2406	2.2259	1.5763	2.4110

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
1B-9_87	0.0561	0.1736	7.7144	3.5740	0.5580	0.4301	8.0388	0.2736	3.7471	3.5725	0.7858	1.2203	0.4999	0.7745
4A-1_87	0.0209	0.0215	1.4845	0.7693	0.1952	0.1286	10.1347	0.9433	17.1529	5.6935	9.7642	2.3584	1.6576	2.5159
3B-1_89	0.0000	0.1154	1.5627	0.9305	0.5224	0.4488	11.7317	0.6475	12.4731	7.7523	7.2473	1.3594	0.8555	2.1724
2C-4_89	0.0000	0.0953	1.6395	1.0319	0.5956	0.5161	11.2912	0.5563	13.0169	8.1396	6.5306	1.3357	0.8831	2.2696
1B-1_89	0.0274	0.1080	4.9752	2.3882	0.3606	0.2963	7.6594	0.4997	2.1145	1.6669	5.8118	0.5411	0.2013	0.3660
1C-2_89	0.0416	0.1395	5.1800	2.4452	0.3904	0.3082	8.2143	0.4793	2.5395	2.0277	6.6359	0.6645	0.2776	0.4343
4C-2_87	0.0219	0.0266	1.5950	0.8198	0.2024	0.1416	10.2979	0.9340	19.3667	5.9908	10.3537	2.4808	1.7511	2.6164
1C-13_89	0.1011	0.3487	14.5537	7.1324	1.2310	0.9534	0.5089	0.0134	0.7004	1.7906	5.2301	0.8197	0.4215	0.7805
3B-17_87	0.0000	1.8939	13.9833	9.7089	6.0403	6.5230	0.0115	0.0000	0.0058	0.0000	0.0000	0.0085	0.1293	1.2312
2B-9_87	0.0000	0.2842	4.9208	3.0281	1.8253	1.5200	6.9170	0.4264	8.8572	7.6017	8.5139	2.7738	1.9959	3.5422
1C-3_87	0.0540	0.1238	3.9286	1.7565	0.2783	0.1955	11.1458	0.4186	3.8171	2.9242	0.6301	0.9159	0.3631	0.5251
4B-9_87	0.0324	0.0366	2.1112	1.0872	0.2750	0.1868	8.5852	0.6128	20.5249	7.0946	11.5660	3.0433	2.1893	3.4010
3B-11_89	0.0000	0.2042	3.0531	1.8718	1.1046	0.9757	7.4097	0.2264	12.2713	10.4801	8.7333	1.9959	1.3471	3.6840
2C-7_89	0.0000	0.1141	1.6864	1.0344	0.5880	0.4940	10.8018	0.4212	13.4291	8.6755	6.5704	1.4979	0.9864	2.4857
1B-14_89	0.1034	0.3635	16.9828	8.5400	1.4134	1.1714	0.0788	0.0000	0.1949	1.0043	3.0506	0.5057	0.2989	0.6920
1A-4_87	0.0638	0.1403	4.2974	1.9044	0.3038	0.2099	11.6166	0.4179	4.0930	3.1919	0.6757	1.0027	0.4055	0.5801
2C-9_87	0.0000	0.2794	4.6402	2.8405	1.6762	1.4161	8.2816	0.4751	9.1698	7.5381	8.5882	2.7643	1.9320	3.4909
2B-9_89	0.0000	0.1396	2.1753	1.3237	0.7477	0.6352	10.0002	0.3326	13.1570	9.8845	7.1507	1.7467	1.1838	3.0174
2B-13_87	0.0000	0.4544	9.4544	6.0680	3.6844	3.1519	0.5608	0.0000	2.3454	5.0504	4.3447	2.4984	2.1942	4.8475

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2B-16_89	0.0000	0.8275	10.1022	6.6555	3.9648	3.5115	0.0063	0.0000	0.0112	0.1960	0.0141	0.2063	0.5075	3.9490
1C-15_89	0.1440	0.4497	17.1662	8.5461	1.4822	1.1668	0.0057	0.0000	0.0475	0.4781	1.2425	0.3355	0.2631	0.6503
1B-1_89	0.0212	0.1119	4.7740	2.2798	0.3423	0.2814	7.3511	0.4808	2.1285	1.6656	5.7342	0.5421	0.1907	0.3656
4B-15_87	0.2651	0.3691	12.0766	7.3249	1.9701	1.4824	0.0075	0.0000	0.0249	0.1345	0.0804	0.2280	0.6841	3.2654
4A-1_87	0.0199	0.0273	1.4909	0.7597	0.1921	0.1264	10.1698	0.9442	17.2605	5.6802	9.6362	2.3258	1.6688	2.5034
3C-3_87	0.0000	0.2629	2.7962	1.6216	0.9591	0.8601	12.7552	0.9194	10.3812	6.9004	8.2430	2.4353	1.5921	2.8416
1C-9_89	0.0422	0.1960	9.2223	4.5371	0.7576	0.5941	6.7770	0.4633	2.5130	2.3599	8.4737	0.7894	0.3341	0.5941
2A-7_89	0.0000	0.1180	2.2624	1.3957	0.8152	0.6946	10.6511	0.4489	13.8062	9.3748	7.0009	1.6157	1.0740	2.9059
3A-9_87	0.0000	0.3335	3.6329	2.1091	1.2491	1.0361	10.2387	0.6184	10.7086	8.0858	9.1605	2.8729	1.9255	3.5310
3B-12_89	0.0000	0.2225	3.3296	2.0385	1.2164	1.0711	5.8170	0.1419	11.3061	10.1488	8.1639	2.0005	1.3975	3.8328
3B-7_89	0.0000	0.1549	2.2561	1.3860	0.8093	0.7322	11.1708	0.5285	13.8674	9.5704	8.8048	1.7354	1.1378	2.9212
1C-14_89	0.0987	0.3711	17.5611	8.7750	1.4993	1.2113	0.0727	0.0000	0.1691	0.9767	2.7629	0.4914	0.2887	0.7139
3A-5_89	0.0000	0.1409	1.7479	1.0258	0.5923	0.5132	11.7989	0.5819	13.6239	8.6877	7.5744	1.5571	1.0122	2.4955
2A-1_87	0.0000	0.1388	2.7931	1.7805	1.0936	0.9727	9.6676	0.7982	7.3644	5.0924	6.3195	1.8024	1.1723	2.2178
3A-17_87	0.0000	1.2523	11.3754	7.0694	4.2330	4.2175	0.0147	0.0000	0.0053	0.2747	0.0506	0.4063	0.8471	3.5921
1A-19_89	0.2585	1.2399	40.3401	23.9702	4.3806	3.7984	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1003
3C-3_87	0.0000	0.2628	2.7435	1.6158	0.9538	0.8576	12.8213	0.9247	10.4692	6.9558	8.2354	2.4389	1.6005	2.8619
4B-4_87	0.0259	0.0315	1.7281	0.8874	0.2238	0.1517	10.3715	0.8994	20.8918	6.3695	10.8245	2.6546	1.8828	2.7997
4B-6_87	0.0290	0.0339	1.8724	0.9718	0.2450	0.1579	9.9840	0.8282	21.9633	6.7110	11.3824	2.8152	2.0007	3.1036

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2B-2_89	0.0000	0.0925	1.8877	1.1896	0.6564	0.5879	11.7566	0.6536	12.6968	8.0967	6.6209	1.3838	0.8931	2.2997
4C-12_87	0.0332	0.0431	2.4671	1.2889	0.3241	0.2207	5.4777	0.2588	15.0488	7.3142	10.6475	3.3138	2.4709	3.9326
3C-8_89	0.0000	0.1550	2.1689	1.2976	0.7569	0.6860	10.3227	0.4474	13.3955	9.2954	8.0764	1.6699	1.0931	2.8409
4B-2_87	0.0224	0.0292	1.6161	0.8328	0.2106	0.1432	10.2368	0.9220	20.5335	6.0007	10.3151	2.4822	1.7527	2.6216
3A-7_89	0.0000	0.1489	2.3470	1.4192	0.8262	0.7468	10.6615	0.4968	13.6499	9.5255	8.4721	1.6976	1.1140	2.9059
2C-15_89	0.0000	0.4967	7.0900	4.6504	2.6765	2.3414	0.0594	0.0000	0.9297	4.1938	1.1945	1.4891	1.5609	6.1363
1B-13_89	0.1185	0.3470	14.7265	7.1445	1.2327	0.9431	0.3816	0.0044	0.5770	1.6848	4.7676	0.7935	0.4135	0.7928
2C-11_87	0.0000	0.2901	7.1511	4.5662	2.8578	2.3923	5.1712	0.3011	7.2261	7.0608	8.3024	2.7877	1.9877	4.0831
3B-16_87	0.0000	1.2642	11.5305	7.1982	4.3104	4.2880	0.0120	0.0000	0.0085	0.2685	0.0550	0.3910	0.8315	3.6201
4C-9_87	0.0231	0.0394	2.2181	1.1459	0.2847	0.1886	9.1229	0.6512	21.7108	7.5654	12.2429	3.2281	2.3229	3.6365
1C-14_87	0.1514	0.3848	13.8269	6.5606	1.0444	0.8209	0.1003	0.0000	0.2832	1.5150	0.2437	0.8389	0.5006	1.0002
2C-13_89	0.0000	0.2482	4.2575	2.6629	1.5353	1.3792	1.9139	0.0112	6.7286	9.2528	4.7920	2.0184	1.5414	4.8209
2C-14_87	0.0000	0.5173	10.0288	6.4816	3.9822	3.3485	0.1789	0.0000	1.1359	3.6401	2.6704	2.0610	2.0684	4.8959
1B-13_89	0.1064	0.3383	15.4006	7.6044	1.2891	1.0113	0.3877	0.0061	0.5614	1.6370	4.6884	0.7647	0.4027	0.7673
2A-10_87	0.0000	0.2879	5.0608	3.1195	1.8713	1.5539	5.9148	0.3506	8.3864	7.2713	8.3388	2.7943	1.9798	3.5438
3A-2_89	0.0011	0.1160	1.5406	0.9134	0.5300	0.4595	11.5085	0.6250	12.5646	7.7427	7.2454	1.3500	0.8863	2.1816
3B-3_87	0.0000	0.2493	2.6351	1.5476	0.9110	0.8087	12.5651	0.9056	10.1934	6.7319	8.0113	2.3583	1.5397	2.7454
1A-5_87	0.0517	0.1423	5.5762	2.5478	0.4167	0.3001	10.0085	0.3540	3.7095	3.1498	0.6895	1.0063	0.4081	0.6260
1B-4_87	0.0569	0.1372	4.1809	1.8665	0.2944	0.2091	11.1413	0.4223	3.9952	3.0761	0.6589	0.9474	0.3554	0.5487

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
4B-16_87	0.3370	0.5656	15.4903	10.2308	2.8366	2.1820	0.0181	0.0000	0.0071	0.0290	0.0152	0.0440	0.2087	1.5168
2B-8_87	0.0000	0.2363	5.3047	3.2896	1.9925	1.6760	7.5828	0.4803	8.4499	7.1344	8.3647	2.6402	1.8451	3.6471
3B-12_87	0.0000	0.4132	4.3078	2.5874	1.4530	1.4080	4.8366	0.1799	8.0067	7.8726	7.9751	3.0306	2.1873	4.0500
3A-5_87	0.0000	0.2716	2.9061	1.6863	0.9985	0.8917	12.1966	0.8700	10.3622	7.0228	8.3737	2.4600	1.6105	2.9353
4C-10_87	0.0311	0.0360	2.2687	1.1721	0.2943	0.1992	7.6763	0.4729	9.5359	7.4814	11.6297	3.2447	2.3723	3.6858
4A-9_87	0.0334	0.0403	2.1996	1.1511	0.2901	0.2014	8.4369	0.5985	20.6274	7.1060	11.4336	3.0478	2.2116	3.4717
3B-8_87	0.0000	0.3305	3.5218	2.0482	1.2122	1.0889	10.3989	0.6482	10.5649	7.8524	8.9919	2.8249	1.8572	3.4075
2B-4_89	0.0000	0.0940	2.0079	1.3290	0.7544	0.6669	10.5574	0.5847	12.0735	8.0404	6.5711	1.3926	0.9103	2.4307
4B-13_87	0.0599	0.0665	3.7153	1.9710	0.4909	0.3567	2.2094	0.0431	9.1594	7.4385	9.1685	3.7379	3.0370	5.1379
3C-17_89	0.0000	0.8387	9.7533	6.6917	4.0233	3.6622	0.0055	0.0000	0.0269	0.4842	0.0536	0.3984	0.7390	4.6407
1C-10_89	0.0539	0.2173	9.1946	4.4354	0.7396	0.5703	5.9925	0.3419	2.5625	2.5937	8.3099	0.9282	0.4031	0.6549
3C-8_89	0.0000	0.1580	2.1113	1.2890	0.7541	0.6546	10.3725	0.4451	13.5506	9.3396	8.2709	1.6858	1.1010	2.8386
1A-13_89	0.0652	0.2945	15.5248	7.9433	1.3006	1.0742	0.7346	0.0169	0.7635	1.6973	5.8669	0.6194	0.2614	0.6765
1C-8_87	0.0452	0.1602	8.8392	4.1869	0.6208	0.4936	8.7256	0.3633	3.5788	3.4234	0.7628	1.1038	0.4408	0.7550
2C-5_87	0.0000	0.1948	4.1343	2.6603	1.6329	1.3265	9.6908	0.7196	8.7425	6.5097	8.0334	2.3410	1.6077	3.0465
2C-7_87	0.0000	0.2177	4.4070	2.7452	1.6838	1.4868	9.5535	0.6566	9.0655	6.8828	8.1390	2.5169	1.7432	3.2105
2A-6_87	0.0000	0.2071	4.3752	2.7845	1.6995	1.4190	8.9211	0.6354	8.5151	6.5137	7.8526	2.3699	1.6643	2.9730
4A-5_87	0.0269	0.0325	1.7654	0.9158	0.2276	0.1596	10.2379	0.8834	19.4406	6.4612	10.9883	2.7019	1.9220	2.8648
2C-12_89	0.0000	0.1884	3.4773	2.1685	1.2617	1.0783	6.0403	0.1332	12.0266	10.4488	7.2220	1.9636	1.4486	3.9550

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
1C-9_87	0.0358	0.1641	9.0367	4.2726	0.6420	0.4841	8.5043	0.3482	3.6451	3.4860	0.7987	1.0998	0.4332	0.7400
1C-18_87	0.3946	1.5426	34.0290	20.1934	3.4707	2.9096	0.0058	0.0000	0.0053	0.0000	0.0000	0.0000	0.0000	0.0579
1B-4_87	0.0666	0.1314	4.1523	1.8459	0.2944	0.2104	11.3532	0.4192	3.9644	3.0925	0.6509	0.9627	0.3814	0.5467
3C-17_87	0.0000	1.6416	13.1061	8.7076	5.2924	5.5891	0.0117	0.0000	0.0055	0.0154	0.0000	0.0505	0.3111	2.0636
3C-13_87	0.0000	0.5772	5.8804	3.4822	2.0557	1.9157	1.4241	0.0210	4.3816	6.8237	5.8759	3.0185	2.3859	4.8471
4C-2_87	0.0193	0.0273	1.5743	0.8056	0.2021	0.1373	10.3853	0.9298	9.3258	6.0101	10.2756	2.4846	1.7524	2.6099
1B-10_87	0.0478	0.1934	10.8891	5.2489	0.7793	0.6267	6.1469	0.2322	3.1239	3.4259	0.8142	1.1526	0.4677	0.8244
1A-14_89	0.0733	0.3280	14.3335	7.1887	1.1813	0.9814	0.2152	0.0000	0.3755	1.3256	4.0270	0.5900	0.3511	0.7179
2A-11_89	0.0000	0.1802	2.9130	1.8352	1.0617	0.8894	7.2217	0.1685	12.9474	10.6383	7.2112	2.0149	1.4343	3.7498
3B-1_87	0.0000	0.2025	2.2054	1.2596	0.7435	0.6531	12.1915	0.9183	9.3391	5.8261	6.9881	2.0402	1.3265	2.3424
2B-16_87	0.0000	1.0443	22.0111	15.5814	10.0602	9.0245	0.0000	0.0000	0.0000	0.0670	0.0187	0.1169	0.5610	3.0215
3A-4_89	0.0000	0.1269	1.7487	1.0495	0.6044	0.4883	11.4881	0.5950	13.0231	8.3733	7.7053	1.4784	0.9691	2.3938
2A-3_87	0.0000	0.1861	3.6932	2.2785	1.3910	1.1504	9.9223	0.7260	8.6038	6.2865	7.5823	2.2219	1.5201	2.8224
3A-8_87	0.0000	0.3329	3.4179	1.9977	1.1868	1.0721	11.2180	0.7039	11.0522	8.0994	9.2479	2.8667	1.8884	3.4436
1A-8_87	0.0513	0.1655	8.2062	3.8812	0.5759	0.4449	8.2877	0.3218	3.5095	3.3479	0.7922	1.1090	0.4113	0.7116
2B-1_89	0.0000	0.0884	1.7153	1.0933	0.5922	0.5222	11.9657	0.6655	12.7899	7.9828	6.3255	1.3578	0.8895	2.2041
1B-4_89	0.0337	0.1422	6.2545	3.0223	0.4907	0.3763	7.8955	0.5066	2.4371	1.9831	6.8262	0.6261	0.2467	0.4494
3A-6_89	0.0000	0.1504	2.0108	1.1997	0.6949	0.6205	11.2985	0.5316	13.8736	9.2483	8.3144	1.6392	1.0998	2.7187
3B-3_89	0.0000	0.1276	1.6172	0.9482	0.5328	0.4692	12.0390	0.6245	13.3617	8.4525	7.7548	1.4625	0.9545	2.3489

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2B-14_89	0.0000	0.4134	6.2372	4.0476	2.3176	2.0071	0.2327	0.0000	2.1331	6.2610	2.3189	1.8348	1.7163	5.9886
1C-7_89	0.0220	0.1692	9.0581	4.5166	0.7112	0.5526	8.1688	0.5872	2.6067	2.2158	8.4175	0.6679	0.2390	0.5276
1C-13_87	0.1051	0.3206	13.8331	6.5917	1.0402	0.8008	0.5371	0.0000	0.8676	2.4374	0.4486	1.0632	0.5488	0.9923
1A-5_87	0.0396	0.1341	6.1509	2.8433	0.4181	0.3176	9.1711	0.3824	3.5371	3.0589	0.7020	1.0010	0.3794	0.6123
3A-10_87	0.0000	0.3434	3.6672	2.1631	1.2638	1.1439	8.5825	0.4659	10.0288	7.9391	8.8015	2.9165	1.9333	3.6011
3C-14_87	0.0000	0.6554	6.5648	3.8869	2.3426	2.2285	0.3956	0.0000	2.0427	5.0608	3.7206	2.5226	2.2590	4.9300
2C-2_87	0.0000	0.1703	3.3880	2.1575	1.2717	1.1847	10.8494	0.9205	8.3426	5.7958	7.1713	2.1615	1.3921	2.5619
4A-11_87	0.0417	0.0484	2.6027	1.3697	0.3445	0.2380	6.3807	0.3435	8.9132	7.5981	11.4336	3.3903	2.5062	4.0080
2C-17_89	0.0000	1.0707	11.5820	8.3001	5.0863	4.6588	0.0069	0.0000	0.0000	0.0053	0.0000	0.0189	0.1391	2.1527
2C-13_89	0.0000	0.2414	4.5120	2.8235	1.6543	1.4464	1.8508	0.0080	6.7704	9.1151	4.8817	1.9821	1.5315	4.7634
3C-19_89	0.0000	1.8610	13.7604	11.4621	7.7679	7.8831	0.0057	0.0000	0.0061	0.0000	0.0000	0.0000	0.0000	0.4155
1C-15_89	0.1276	0.4431	18.0738	9.0709	1.5648	1.2531	0.0056	0.0000	0.0305	0.4884	1.2588	0.3226	0.2447	0.6639
1C-5_87	0.0519	0.1421	5.1666	2.3376	0.3662	0.2710	10.2743	0.3658	3.7181	3.0872	0.6873	0.9901	0.4185	0.6062
1B-15_89	0.1429	0.4801	20.4276	10.3595	1.7846	1.4247	0.0000	0.0000	0.0079	0.3194	0.8326	0.2309	0.1889	0.5958
2A-1_87	0.0000	0.1379	2.6370	1.6466	1.0207	0.8771	9.9562	0.7910	7.6306	5.1886	6.3384	1.8583	1.2180	2.1859
2A-15_87	0.0000	0.6140	14.0001	9.2517	5.7580	4.9751	0.0533	0.0000	0.4352	2.4392	1.5779	1.6996	1.8850	5.1381
1A-18_87	0.3825	1.1394	22.1502	11.9250	2.0228	1.5982	0.0100	0.0000	0.0070	0.0000	0.0000	0.0039	0.0046	0.1338
1C-16_89	0.1235	0.5865	30.5276	16.4997	2.9959	2.4478	0.0000	0.0000	0.0000	0.0335	0.1638	0.0830	0.0550	0.4620
1C-4_89	0.0277	0.1301	6.3896	3.0702	0.4642	0.3821	8.3772	0.5714	2.4729	2.0109	7.0772	0.6341	0.2602	0.4592

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
1B-8_87	0.0471	0.1619	8.7739	4.1885	0.6297	0.5014	8.9554	0.3861	3.6390	3.3764	0.8116	1.1066	0.4155	0.7157
2C-8_87	0.0000	0.2345	4.0750	2.4830	1.4903	1.2305	7.2312	0.5080	8.7686	6.9378	8.0939	2.4927	1.7353	3.1330
1A-14_89	0.1066	0.3505	13.9686	6.8469	1.1772	0.9187	0.1957	0.0000	0.3924	1.3976	3.7995	0.7023	0.3909	0.7486
2C-5_87	0.0026	0.1907	4.3553	2.8682	1.7579	1.4487	10.3429	0.8484	8.6821	6.4015	8.1668	2.3652	1.6686	2.8964
3B-12_89	0.0000	0.2281	2.9691	1.7820	1.0319	0.9403	6.6028	0.1568	12.4343	10.7347	8.4626	2.0693	1.4677	3.8099
3A-16_89	0.0000	0.7444	9.2487	6.2966	3.7921	3.4203	0.0000	0.0000	0.1034	1.1419	0.2015	0.6692	1.0000	5.3419
3A-12_89	0.0000	0.2339	3.2319	1.9651	1.1511	1.0376	6.0908	0.1418	7.9537	10.5344	8.2747	2.0691	1.4701	3.9382
1C-19_87	0.3464	3.0852	51.9451	43.5418	8.7954	9.2032	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3B-17_89	0.0000	1.2601	12.1286	8.5755	5.3051	4.8206	0.0000	0.0000	0.0000	0.0127	0.0000	0.0446	0.1989	2.5077
3B-14_87	0.0000	0.7610	7.3593	4.3840	2.6336	2.7423	0.1938	0.0000	1.3711	4.3458	2.8916	2.3661	2.2702	5.1968
2C-12_87	0.0000	0.3515	6.4621	4.0270	2.4355	2.0157	4.4589	0.1845	7.2471	7.4618	8.0984	2.9488	2.1971	4.1779
3A-11_87	0.0000	0.3906	4.0820	2.4036	1.4144	1.2876	6.9955	0.3293	9.4973	8.2071	8.6935	3.0617	2.1274	3.9642
1C-10_87	0.0409	0.2010	9.7377	4.6412	0.6957	0.5334	6.9301	0.2369	3.4450	3.6424	0.8162	1.2739	0.4987	0.8412
2C-19_87	0.0000	2.1724	22.2321	19.6465	13.6034	14.9285	0.0049	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1000
1B-9_87	0.0561	0.1735	8.2358	3.8399	0.5873	0.4541	8.1976	0.2840	3.6341	3.5037	0.8007	1.1604	0.4626	0.7749
2C-17_87	0.0000	1.1432	20.3457	14.3038	9.2353	8.2902	0.0000	0.0000	0.0000	0.0136	0.0000	0.0717	0.4135	2.5685
1C-18_89	0.3515	1.9164	47.3933	30.8762	5.8226	5.3130	0.0079	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0199
4B-15_87	0.2738	0.3695	12.1624	7.3734	1.9961	1.4806	0.0194	0.0000	0.0246	0.1406	0.0781	0.2298	0.6892	3.2879
1C-1_89	0.0372	0.1174	4.0415	1.8793	0.3038	0.2338	8.4051	0.4593	2.3027	1.7423	5.7817	0.5703	0.2350	0.3592

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2B-3_87	0.0000	0.1867	4.0397	2.7050	1.5631	1.4386	11.4118	1.0166	8.6870	6.1161	8.1131	2.3406	1.5374	2.8315
2B-9_87	0.0000	0.2728	5.6239	3.5263	2.1500	1.8927	7.2971	0.4613	8.4766	7.2525	8.4113	2.7026	1.9210	3.7036
4C-11_87	0.0338	0.0421	2.3951	1.2381	0.3143	0.2097	6.6103	0.3595	16.6267	7.4759	11.2959	3.3037	2.4469	3.8141
3A-6_89	0.0000	0.1479	2.0997	1.2583	0.7296	0.6361	11.1330	0.5306	13.6227	9.1960	8.3116	1.6318	1.0815	2.7356
1B-17_89	0.1860	0.8837	37.8246	21.9260	3.9672	3.4651	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1491
1B-13_89	0.1273	0.3474	12.6599	6.0803	1.0390	0.7945	0.4152	0.0091	0.6597	1.7677	4.6710	0.8276	0.4275	0.7962
3B-14_87	0.0000	0.7544	7.4762	4.4709	2.6542	2.6038	0.1997	0.0000	1.3459	4.3660	2.9171	2.3862	2.2974	5.3358
2C-13_87	0.0000	0.4012	8.0986	5.1535	3.1176	2.6462	1.1681	0.0289	3.7092	5.9995	5.4207	2.7149	2.1961	4.5851
3A-13_87	0.0000	0.5687	5.8106	3.3952	2.0349	1.8400	1.6495	0.0262	4.6861	6.9519	6.1122	3.0089	2.3930	4.8161
3A-12_89	0.0000	0.2322	3.2909	2.0113	1.1889	1.0633	6.0664	0.1478	11.8360	10.4857	8.3752	2.0497	1.4309	3.9301
3C-7_89	0.0000	0.1466	2.1276	1.2775	0.7320	0.6683	10.5633	0.4917	13.4307	9.1084	8.2756	1.6409	1.0828	2.7680
1B-18_89	0.3609	5.6923	43.0690	50.8939	11.8741	15.5092	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0063
3A-5_89	0.0000	0.1372	1.7865	1.0643	0.6096	0.5429	11.7296	0.5761	13.6453	8.8198	7.9303	1.5367	1.0191	2.5258
1A-18_89	0.2346	0.8205	26.6402	14.1730	2.5123	2.0348	0.0074	0.0000	0.0056	0.0000	0.0100	0.0239	0.0470	0.2944
2A-3_89	0.0000	0.0949	1.8416	1.1579	0.6626	0.6033	11.3110	0.6019	12.9401	8.2312	6.4412	1.3839	0.9370	2.3461
2A-10_89	0.0000	0.1505	2.8011	1.7194	0.9778	0.8902	8.8197	0.2812	14.0932	10.6006	7.5205	2.0318	1.5296	3.5647
2A-2_87	0.0000	0.1825	3.9761	2.5409	1.5732	1.3595	10.5042	0.8472	8.5339	6.0840	7.6601	2.2240	1.5180	2.7439
2A-1_87	0.0000	0.1352	2.7674	1.7772	1.0434	0.8769	10.3589	0.8754	7.4525	4.9925	6.3161	1.8640	1.1765	2.0715
3A-15_89	0.0000	0.5331	7.0907	4.5148	2.6944	2.4011	0.1026	0.0000	1.2215	4.7997	1.8233	1.5964	1.6386	5.9844

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
1C-18_87	0.3619	1.5217	36.8386	22.1954	3.8574	3.2546	0.0055	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0562
1C-6_87	0.0467	0.1448	6.5233	3.0364	0.4673	0.3552	9.6034	0.3931	3.6910	3.2467	0.7508	1.0439	0.4009	0.6499
1A-11_87	0.0722	0.2199	10.9165	5.1828	0.8240	0.6546	4.7863	0.1378	2.8867	3.5804	0.7711	1.2848	0.5548	0.9088
1C-2_89	0.0420	0.1390	5.1288	2.4243	0.3875	0.3103	8.6047	0.4888	2.6409	1.9831	6.6993	0.6645	0.2762	0.4314
4A-6_87	0.0291	0.0355	1.8597	0.9767	0.2463	0.1729	9.8708	0.8068	20.2669	6.6816	11.1505	2.7994	1.9965	3.0605
2C-7_89	0.0000	0.1126	1.8362	1.1118	0.6327	0.5567	10.4941	0.4132	13.1355	8.6660	6.5976	1.4833	0.9991	2.5781
2A-15_87	0.0000	0.6132	12.3554	8.1695	5.0292	4.2593	0.0538	0.0000	0.4629	2.4553	1.5713	1.7069	1.9080	4.9634
1A-19_87	0.3539	2.1450	43.4426	29.9942	5.6427	5.1507	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2B-18_89	0.0000	1.7875	12.8472	11.5296	7.9668	8.4016	0.0064	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2223
1C-15_87	0.1469	0.4368	17.9013	8.7569	1.4434	1.0960	0.0073	0.0000	0.0601	0.7048	0.1056	0.5030	0.3646	0.8630
1A-17_87	0.2074	0.7056	25.4600	13.3674	2.2464	1.8138	0.0000	0.0000	0.0000	0.0057	0.0000	0.0436	0.0541	0.3974
3C-18_87	0.0000	2.3893	14.6962	11.1853	7.3114	7.7873	0.0172	0.0000	0.0053	0.0000	0.0000	0.0000	0.0058	0.4167
4C-10_87	0.0351	0.0419	2.2827	1.1796	0.2965	0.1924	7.7030	0.4859	9.4769	7.4392	11.6301	3.2493	2.3700	3.7396
2C-14_87	0.0000	0.5216	10.1247	6.4737	3.9619	3.3713	0.1666	0.0000	1.0536	3.6363	2.6965	2.0817	2.0770	4.8882
1B-6_87	0.0455	0.1462	5.9805	2.7466	0.4309	0.3226	9.8269	0.3758	3.7552	3.1957	0.7318	1.0387	0.4067	0.6284
3B-18_89	0.0000	1.8072	14.0994	11.8108	8.0568	8.3707	0.0054	0.0000	0.0062	0.0000	0.0000	0.0000	0.0018	0.5440
2A-1_89	0.0000	0.0907	1.5604	0.9537	0.5403	0.4773	11.9613	0.6088	13.1647	8.0070	6.3209	1.3593	0.8690	2.2167
1A-3_87	0.0555	0.1302	4.0607	1.8169	0.2742	0.2045	11.4913	0.4334	3.9634	3.0446	0.6474	0.9542	0.3786	0.5533
3C-9_87	0.0000	0.3187	3.4163	2.0144	1.1414	1.0431	9.2871	0.5528	10.0593	7.5691	8.4959	2.7110	1.8097	3.3264

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
1C-17_89	0.2322	0.9242	31.1223	17.2692	3.0682	2.5464	0.0000	0.0000	0.0000	0.0000	0.0000	0.0110	0.0169	0.2197
4B-7_87	0.0299	0.0354	1.9930	1.0344	0.2550	0.1710	9.5001	0.7435	20.8851	6.9445	11.4409	2.9287	2.0865	3.2551
3C-4_87	0.0000	0.2563	2.7736	1.6144	0.9558	0.7875	12.3597	0.8726	10.4395	6.9140	8.1568	2.4350	1.5786	2.8301
4B-3_87	0.0226	0.0280	1.6322	0.8386	0.2137	0.1365	10.3816	0.9202	20.4970	6.1901	10.5446	2.5718	1.8114	2.7117
1C-5_87	0.0439	0.1290	5.6211	2.5755	0.4030	0.2997	9.6663	0.4038	3.6211	2.9994	0.6968	0.9619	0.3727	0.5912
3C-12_89	0.0000	0.2041	3.0585	1.8666	1.1056	0.9895	6.1504	0.1614	11.3619	9.7614	7.9288	1.8790	1.3342	3.5574
3B-14_89	0.0000	0.4247	5.9286	3.7517	2.2338	1.9709	0.5084	0.0000	3.3141	7.4991	3.7360	2.0441	1.7809	5.7842
2A-18_89	0.0000	1.4007	14.6374	11.7337	7.5757	7.6241	0.0000	0.0000	0.0078	0.0000	0.0000	0.0000	0.0056	0.7936
3C-2_89	0.0000	0.1125	1.5587	0.9358	0.5443	0.4618	11.5400	0.6232	12.2459	7.7642	7.2073	1.3381	0.8663	2.1623
2C-10_87	0.0000	0.2755	4.9878	3.1632	1.9414	1.5948	5.8391	0.3670	8.2794	7.3148	8.0545	2.7376	1.9361	3.6504
1A-9_87	0.0525	0.1730	8.9541	4.2585	0.6204	0.4781	8.1573	0.3281	3.5517	3.4743	0.8249	1.1717	0.4448	0.7827
2B-7_87	0.0000	0.2345	5.8252	3.7249	2.2778	1.9827	7.6993	0.5639	7.9379	6.4973	8.1723	2.4991	1.7553	3.3371
3A-2_89	0.0000	0.1151	1.5359	0.9096	0.5144	0.4302	11.2579	0.6078	12.4640	7.7177	7.2008	1.3393	0.8721	2.1841
4C-10_87	0.0347	0.0402	2.2845	1.1808	0.2925	0.2001	7.7220	0.4755	9.4570	7.4754	11.6570	3.2486	2.3539	3.7321
1B-10_87	0.0588	0.1904	10.4193	5.0021	0.7392	0.5995	6.7758	0.2356	3.2854	3.4810	0.8110	1.1932	0.4718	0.8324
3B-2_87	0.0000	0.2285	2.4207	1.4071	0.8303	0.7575	12.1278	0.8874	9.7737	6.2913	7.5130	2.2177	1.4781	2.5827
2A-7_89	0.0000	0.1196	2.1740	1.3300	0.7744	0.6547	10.7398	0.4450	13.8643	9.2454	7.1738	1.6001	1.0883	2.7762
1A-6_87	0.0507	0.1458	6.7204	3.1004	0.4824	0.3626	8.9079	0.3637	3.5829	3.1667	0.7396	1.0385	0.4194	0.6650
3B-9_87	0.0000	0.3526	3.7187	2.1661	1.2733	1.1163	10.2314	0.5996	10.9231	8.3743	9.4033	3.0279	2.0091	3.6761

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2C-5_87	0.0000	0.1993	3.8999	2.3960	1.4690	1.2144	9.8562	0.7019	8.9619	6.6189	7.8855	2.3553	1.6095	2.9706
1A-5_89	0.0490	0.1490	6.0168	2.8432	0.4650	0.3677	8.0028	0.4750	2.6562	2.1463	7.0270	0.7259	0.2818	0.4835
2B-11_89	0.0000	0.1718	2.8553	1.8159	1.0398	0.8940	6.2202	0.1462	11.7194	9.8435	6.7308	1.8191	1.3172	3.5419
3C-15_89	0.0000	0.4737	7.4363	4.7234	2.8247	2.5520	0.2306	0.0000	2.0091	6.0296	2.7444	1.8399	1.6822	6.0305
1C-7_89	0.0468	0.1793	7.5118	3.6486	0.5903	0.4606	7.7245	0.4890	2.6353	2.3083	7.8066	0.7884	0.3120	0.5475
2C-6_87	0.0000	0.2161	4.5296	2.8006	1.7257	1.4737	8.9043	0.6507	8.6353	6.6696	8.0400	2.4288	1.6618	3.0895
4A-4_87	0.0291	0.0322	1.6982	0.8823	0.2264	0.1535	10.3568	0.9085	9.5930	6.3425	10.8233	2.6402	1.8655	2.7996
2C-15_89	0.0000	0.5006	6.4851	4.1878	2.3846	2.0731	0.0595	0.0000	0.9847	4.2602	1.2208	1.5093	1.5947	6.0776
3B-13_87	0.0000	0.6137	6.1972	3.6559	2.1810	1.9998	0.9274	0.0112	3.5203	6.3937	5.2643	2.9440	2.4417	5.0381
1A-9_89	0.0566	0.1952	8.3904	4.0563	0.6739	0.5179	7.0303	0.3899	2.6737	2.5028	8.2184	0.8528	0.3520	0.5892
1A-2_89	0.0362	0.1251	4.6920	2.1961	0.3481	0.2658	8.3054	0.4880	2.4696	1.8861	6.3883	0.6122	0.2323	0.3929
3C-6_89	0.0000	0.1390	2.0301	1.2267	0.7163	0.6162	10.5491	0.5210	12.6294	8.6198	7.8307	1.5325	1.0114	2.5979
3B-5_87	0.0000	0.2645	2.8323	1.6574	0.9898	0.9021	12.2045	0.8616	10.3982	7.0410	8.4128	2.4830	1.6559	2.9152
1B-6_89	0.0536	0.1724	6.4974	3.0480	0.5187	0.3817	7.9726	0.4492	2.8133	2.3387	7.6798	0.7933	0.3356	0.5265
3C-2_87	0.0000	0.2395	2.5284	1.4971	0.8827	0.8036	12.1011	0.8893	9.8096	6.3627	7.6162	2.2190	1.4651	2.6062
1A-15_89	0.1169	0.3909	16.4384	8.1906	1.3770	1.1049	0.0529	0.0000	0.1480	0.9049	2.4351	0.4952	0.2903	0.7207
3B-15_87	0.0000	0.9232	9.0769	5.4290	3.2054	3.1768	0.0280	0.0000	0.2809	2.1140	1.0477	1.5302	1.8355	5.1336
4A-5_87	0.0272	0.0287	1.7557	0.9113	0.2325	0.1533	10.2013	0.8769	9.9062	6.4765	10.9361	2.7075	1.9249	2.9509
1A-12_89	0.0757	0.2497	10.9555	5.3017	0.8880	0.6875	3.5189	0.1820	2.0381	2.5214	7.9573	0.9529	0.4352	0.7066

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
4C-8_87	0.0213	0.0363	2.0455	1.0626	0.2635	0.1697	9.3257	0.6962	10.1583	7.1919	11.7044	3.0520	2.1852	3.4046
2A-9_87	0.0000	0.2641	4.8491	2.9875	1.7783	1.4739	7.7042	0.4536	8.7260	7.3750	8.4982	2.7238	1.9075	3.4489
2B-13_89	0.0000	0.3110	5.0398	3.1511	1.8268	1.5799	1.3295	0.0000	5.7506	9.2976	4.4206	2.1272	1.7750	5.5022
2B-11_87	0.0000	0.3351	5.6209	3.4716	2.0890	1.7395	4.4726	0.1714	7.1825	7.4025	7.7324	2.8771	2.0885	3.9468
2B-8_89	0.0000	0.1389	2.1389	1.3340	0.7649	0.6527	10.9644	0.3981	14.7162	9.8946	7.4102	1.7418	1.1839	2.9936
4C-15_87	0.1154	0.1193	5.7217	3.0788	0.7788	0.5643	0.1568	0.0000	1.7290	4.4460	3.6993	3.0307	3.0937	6.2661
3C-10_89	0.0000	0.1765	2.6833	1.6617	0.9804	0.8820	8.5060	0.3252	12.6140	9.6716	8.2613	1.8143	1.2356	3.2267
3C-10_87	0.0000	0.3402	3.6583	2.1213	1.2500	1.1467	7.9414	0.4215	9.4840	7.6321	8.4312	2.7929	1.9007	3.5069
2A-5_89	0.0000	0.1126	1.8467	1.1482	0.6611	0.5675	12.6243	0.5542	14.5154	9.1309	7.1278	1.5548	1.0366	2.5827
4A-10_87	0.0441	0.0481	2.3868	1.2312	0.3118	0.2222	7.5422	0.4801	11.5905	7.6126	11.6171	3.3048	2.4170	3.7850
2C-8_89	0.0000	0.1125	1.7739	1.1045	0.6385	0.5499	9.8530	0.3786	11.9163	8.6186	6.4454	1.5045	1.0044	2.5486
3C-9_89	0.0000	0.1611	2.3960	1.4503	0.8438	0.7566	9.6272	0.4047	13.0640	9.5275	8.4563	1.7176	1.1639	3.0127
2B-9_87	0.0000	0.2810	5.2606	3.2803	1.9852	1.6439	7.5301	0.4296	8.7513	7.4207	8.3197	2.7535	1.9351	3.5600
3C-16_87	0.0000	1.2054	10.8470	6.7838	4.0436	4.1706	0.0093	0.0000	0.0181	0.4193	0.1180	0.5242	1.0200	3.6243
3A-1_89	0.0000	0.1120	1.5101	0.8955	0.5022	0.4518	10.8890	0.5895	11.9247	7.4575	6.9638	1.3110	0.8501	2.1291
3A-12_87	0.0000	0.4049	4.1988	2.4508	1.4697	1.3044	5.5642	0.2271	8.5008	7.9400	8.1813	3.0203	2.1476	4.0300
3B-15_87	0.0000	0.9342	8.9002	5.3700	3.2018	3.1492	0.0273	0.0000	0.2879	2.1046	1.0485	1.5218	1.8357	4.9760
2B-15_89	0.0000	0.5134	7.4569	4.9087	2.8586	2.4462	0.0099	0.0000	0.4572	2.7314	0.6430	1.1275	1.3302	5.8131
1B-11_89	0.0778	0.2500	9.9929	4.8139	0.8163	0.6201	3.8118	0.1921	2.1319	2.5704	7.9923	0.9469	0.4377	0.6978

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2C-15_89	0.0000	0.4905	7.3586	4.6903	2.7174	2.4015	0.0604	0.0000	0.9309	4.2295	1.1991	1.4571	1.5970	6.2080
2A-6_87	0.0000	0.2100	4.4457	2.8423	1.7539	1.4384	8.8657	0.6498	8.3175	6.3938	7.8802	2.3450	1.6593	3.1223
4C-7_87	0.0251	0.0341	1.9471	0.9950	0.2460	0.1684	9.7004	0.7635	10.1878	6.9356	11.6024	2.9373	2.0878	3.2528
1B-5_87	0.0405	0.1353	6.2642	2.8949	0.4499	0.3365	9.1262	0.3922	3.4418	2.9965	0.6880	0.9596	0.3460	0.5923
2B-15_87	0.0000	0.7893	14.0146	9.1408	5.7170	4.9418	0.0107	0.0046	0.1198	1.1562	0.4924	1.0701	1.5218	4.6530
3C-17_89	0.0000	0.8513	8.9707	6.0762	3.6350	3.2064	0.0073	0.0000	0.0167	0.4836	0.0539	0.3890	0.7400	4.5700
4B-7_87	0.0310	0.0343	1.9844	1.0200	0.2569	0.1708	9.4193	0.7479	21.1102	6.8416	11.4231	2.8940	2.0727	3.2260
2B-9_89	0.0000	0.1397	2.1542	1.3083	0.7358	0.6570	9.8470	0.3323	14.1207	9.7916	7.1057	1.7481	1.1616	2.9797
1B-14_87	0.1126	0.3384	15.2415	7.3669	1.1803	0.9116	0.2382	0.0000	0.5175	1.9569	0.3469	0.9128	0.5065	0.9907
3B-18_89	0.0000	1.8403	12.7631	10.5018	7.0937	7.2937	0.0060	0.0000	0.0000	0.0000	0.0000	0.0000	0.0038	0.5319
3C-11_87	0.0000	0.3679	3.9640	2.3287	1.3711	1.3203	6.5830	0.3018	9.0130	7.9277	8.3622	2.9564	2.0708	3.7834
2B-14_87	0.0000	0.5478	13.0088	8.8314	5.4577	4.7226	0.1139	0.0000	0.6767	3.0666	2.2454	1.9418	1.9510	4.9783
2A-13_87	0.0000	0.4209	8.4407	5.3374	3.3048	2.7393	1.2023	0.0296	3.8715	6.2225	5.6816	2.8769	2.2796	4.7610
2A-14_87	0.0000	0.5305	10.5553	6.8485	4.1768	3.5842	0.3235	0.0000	1.6705	4.5520	3.6450	2.4219	2.2796	5.2114
2B-2_89	0.0000	0.0958	1.6615	1.0456	0.5935	0.5139	12.5145	0.6460	14.3141	8.3130	6.7829	1.4025	0.9121	2.2494
1B-18_87	0.2710	0.8597	26.0105	13.7414	2.3301	1.8353	0.0067	0.0000	0.0000	0.0000	0.0000	0.0181	0.0318	0.3154
3B-10_87	0.0000	0.3478	3.7695	2.2141	1.2948	1.2913	7.9261	0.4074	9.6588	7.8780	8.5623	2.8756	1.9795	3.5855
4C-7_87	0.0280	0.0264	1.9415	1.0085	0.2563	0.1698	9.6966	0.7628	22.5212	6.9771	11.6081	2.9365	2.0946	3.2513
1C-9_87	0.0498	0.1715	9.7078	4.6707	0.6932	0.5557	7.6783	0.3185	3.3880	3.3989	0.8064	1.0904	0.4092	0.7630

Sample	Di-aromatic A	Di-aromatic B	C10-monoaromatics A	C10-monoaromatics B	C11/C12-monoaromatics A	C11/C12-monoaromatics B	C6-alkanes A	C6-monoaromatics	C7-alkanes A	C7-alkanes B	C7-monoaromatics	C8-alkanes A	C8-alkanes B	C8-alkanes C
2B-12_89	0.0000	0.1796	3.1130	1.9754	1.1349	0.9511	4.8535	0.0869	9.9062	9.7175	6.3682	1.9031	1.4043	3.7654
1A-4_89	0.0380	0.1362	5.6911	2.6967	0.4379	0.3360	7.7680	0.4798	2.5141	2.0223	6.6367	0.6767	0.2596	0.4418
1B-18_87	0.2442	0.8223	28.2187	15.0286	2.5408	2.0409	0.0000	0.0000	0.0000	0.0000	0.0000	0.0213	0.0235	0.3029
1A-4_87	0.0688	0.1358	4.2841	1.9014	0.3037	0.2187	11.4960	0.4252	4.0897	3.1767	0.6733	0.9972	0.4059	0.5784
3B-1_89	0.0000	0.1176	1.4796	0.8721	0.4868	0.4167	11.7968	0.6569	12.6995	7.7743	7.2195	1.3481	0.8607	2.1413
1A-12_87	0.0540	0.2309	11.5659	5.4833	0.8703	0.6574	3.8353	0.1117	2.5482	3.5034	0.7613	1.2545	0.5509	0.9590
2B-11_87	0.0000	0.3332	6.0543	3.7681	2.2759	1.8872	3.9687	0.1741	6.9699	7.1248	7.7603	2.8627	2.1356	4.0296
3A-9_87	0.0000	0.3343	3.5826	2.0785	1.2274	1.0955	10.2760	0.6217	10.7205	8.0579	9.1098	2.9083	1.9308	3.5489
4A-10_87	0.0392	0.0463	2.4118	1.2679	0.3208	0.2205	7.5984	0.4740	9.6493	7.5863	11.8380	3.3017	2.4139	3.8157
4B-12_87	0.0422	0.0472	2.6224	1.3636	0.3423	0.2336	5.5783	0.2678	15.4212	7.4930	11.0448	3.3779	2.5361	4.0395
4A-13_87	0.0677	0.0772	3.8293	2.0322	0.5370	0.3763	1.6988	0.0282	8.0287	7.2025	8.5382	3.7104	3.0573	5.2558
3C-12_87	0.0000	0.3746	3.9660	2.3477	1.3862	1.2385	4.3920	0.1959	7.5690	7.2099	7.4051	2.7563	1.9667	3.6956
2C-17_89	0.0000	1.0763	11.3814	8.1096	4.9715	4.4942	0.0067	0.0000	0.0000	0.0048	0.0000	0.0445	0.1319	2.1267
3A-3_87	0.0000	0.2439	2.6473	1.5320	0.8975	0.8064	12.8017	0.9203	10.2437	6.7216	8.0084	2.3836	1.5489	2.7501
3C-17_89	0.0000	0.8449	9.3742	6.3570	3.8332	3.4054	0.0066	0.0000	0.0103	0.4756	0.0534	0.3955	0.7259	4.6111
2B-1_89	0.0000	0.0881	1.7546	1.1074	0.6399	0.5685	11.5512	0.6064	12.5694	7.8635	6.2561	1.3388	0.8698	2.2450
4A-8_87	0.0329	0.0386	2.0019	1.0438	0.2631	0.1882	8.9154	0.6475	9.5835	6.9314	11.1805	2.9673	2.1247	3.2734
1A-16_89	0.1673	0.5247	19.9416	10.0762	1.7422	1.3881	0.0000	0.0000	0.0074	0.3109	0.7059	0.2387	0.1990	0.6253

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2C-1_89	6.8330	2.0546	1.2083	2.0690	3.2577	2.9319	2.3879	2.0947	1.1942	0.0197	0.0323	0.0049
3C-13_87	14.6087	4.6265	3.1385	3.4739	8.5925	8.2981	4.3286	4.7734	2.3621	0.0117	0.1536	0.0136
3C-3_89	8.4773	2.5229	1.2405	2.1420	3.4189	3.1986	2.4839	2.1386	1.2175	0.0196	0.0544	0.0071
2C-10_87	13.7646	4.2601	2.2680	2.8817	8.6358	8.7021	3.8017	5.0558	2.6056	0.0000	0.0443	0.0000
3C-14_89	16.2627	5.3188	3.1935	5.8663	9.2708	9.0769	7.0971	6.5095	4.0836	0.3489	0.1455	0.0522
1A-7_87	24.4255	8.6021	0.2141	0.0581	15.7008	14.1928	0.0194	0.0000	0.0000	0.0000	0.0720	0.0659
3B-13_89	15.5765	4.9666	2.7738	5.0242	8.1402	7.8499	6.0027	5.4829	3.5444	0.3191	0.1284	0.0365
4C-13_87	16.6684	5.2807	3.1248	1.6523	10.1220	4.9668	3.1263	0.9503	0.1973	0.0000	0.0544	0.0073
3A-15_89	15.7466	5.5081	3.7630	7.3560	11.2520	11.3654	9.1483	8.5189	5.2017	0.3998	0.1995	0.0704
4B-6_87	10.9141	3.2931	1.8176	0.8767	5.6000	4.5900	1.6790	0.4444	0.0601	0.0000	0.0225	0.0000
2C-18_87	0.2614	0.3022	1.4165	4.7396	10.0419	17.5896	11.2488	24.0711	16.1854	0.6790	0.3879	0.1600
4A-4_87	10.2917	3.0984	1.6716	0.8271	5.2517	4.2914	1.5451	0.3363	0.0316	0.0000	0.0192	0.0000
2C-18_87	0.2548	0.2919	1.3739	4.5469	9.0957	15.6967	10.4850	21.9164	14.1986	0.5695	0.3904	0.1477
2A-19_87	0.0076	0.0273	0.4834	2.6906	5.0994	12.2348	9.4142	28.8582	23.0519	0.9878	0.5520	0.2341
2A-16_87	9.6395	4.0342	3.9291	5.5809	15.2957	17.1178	8.2209	11.4224	6.3723	0.2257	0.1717	0.0479

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2B-3_89	7.4710	2.2420	1.2277	2.2783	3.5642	3.2240	2.6761	2.3876	1.4466	0.0510	0.0313	0.0022
4A-17_87	8.1078	4.0272	4.6942	3.6563	20.6210	21.4218	8.6992	3.1731	1.5091	0.1103	0.2396	0.1258
2B-10_87	12.8986	3.9342	2.4695	2.5817	7.2022	6.8797	3.2115	3.7773	1.8406	0.0201	0.0632	0.0054
3A-5_87	9.3986	2.7719	1.6479	1.7676	4.4474	4.1954	2.1636	2.4404	1.1357	0.0000	0.0656	0.0000
1A-7_89	23.7803	8.0590	0.1718	0.0815	14.9494	13.6813	0.0224	0.0000	0.0000	0.0000	0.1005	0.0763
1B-10_87	29.8949	10.8170	0.2599	0.0606	21.2860	19.8538	0.0267	0.0000	0.0000	0.0000	0.0796	0.0620
2B-17_89	1.1690	0.8191	2.5133	8.7092	9.7600	13.2901	15.0816	18.2297	11.8102	0.8604	0.3173	0.1650
3B-10_87	11.5641	3.4430	2.1492	2.2538	5.7107	5.4006	2.8004	3.0811	1.4731	0.0053	0.0955	0.0060
1A-12_87	33.7888	12.3795	0.2974	0.1269	25.0569	23.3781	0.0330	0.0000	0.0000	0.0000	0.1198	0.1077
1B-19_87	3.7079	3.1151	0.1552	0.2409	35.2413	49.3346	0.0911	0.0000	0.0124	0.0000	0.6491	0.6316
3C-11_87	11.8845	3.5771	2.2765	2.3785	6.0202	5.6838	2.9148	3.2026	1.5398	0.0081	0.0930	0.0027
3A-6_87	9.8771	2.9058	1.7717	1.8817	4.6949	4.4213	2.3046	2.5484	1.2132	0.0051	0.0833	0.0044
1A-1_89	17.6169	5.8959	0.1039	0.0242	10.5844	9.7029	0.0139	0.0000	0.0000	0.0000	0.0623	0.0306
1A-4_87	17.9654	6.1630	0.1790	0.0741	10.4150	9.1867	0.0176	0.0000	0.0000	0.0000	0.0796	0.0548
1A-15_87	27.1617	11.4625	0.4035	0.2053	30.7450	30.4348	0.0493	0.0000	0.0000	0.0000	0.2169	0.1940
1C-4_87	19.8514	6.9769	0.1820	0.0748	12.7699	11.5404	0.0176	0.0000	0.0000	0.0000	0.0606	0.0541
3C-9_87	10.5855	3.1409	1.9350	2.0582	5.1505	4.8763	2.5457	2.8479	1.3607	0.0000	0.0819	0.0000
2B-2_89	7.1646	2.1341	1.2150	2.1921	3.3926	3.0372	2.5725	2.2555	1.4172	0.0949	0.0305	0.0066
1B-19_87	3.5325	2.9059	0.2013	0.2463	31.4600	44.7336	0.0881	0.0239	0.0086	0.0000	0.6519	0.6964

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2B-10_87	14.2018	4.3790	2.4318	2.9221	8.7347	8.6263	3.8289	4.8559	2.6102	0.0000	0.0474	0.0000
4A-14_87	18.0977	5.9659	3.8660	2.1083	12.7073	10.9177	4.1097	1.2817	0.3243	0.0000	0.0701	0.0220
3A-6_87	9.8830	2.9092	1.8181	1.8546	4.6854	4.4236	2.3593	2.5964	1.2260	0.0000	0.0807	0.0046
4C-3_87	9.8393	2.9618	1.5609	0.7800	5.0114	4.0404	1.4749	0.3517	0.0309	0.0000	0.0210	0.0000
4B-1_87	8.8864	2.6707	1.4458	0.7066	4.5214	3.6689	1.3456	0.3057	0.0385	0.0000	0.0337	0.0000
4C-5_87	10.4228	3.1440	1.6972	0.8368	5.3912	4.3552	1.6044	0.3863	0.0516	0.0000	0.0303	0.0000
3C-17_87	3.2838	1.7683	2.8429	5.1213	10.9999	13.7888	8.1503	11.5832	6.2627	0.2384	0.4507	0.1135
3B-17_89	2.6087	1.5868	3.0386	9.3296	11.6926	15.4152	15.2776	18.3083	12.4167	0.9666	0.4671	0.1851
1B-17_87	17.4227	8.7608	0.3758	0.2316	33.4038	36.1318	0.0635	0.0000	0.0143	0.0000	0.3156	0.2691
2C-8_89	7.4771	2.2303	1.2983	2.2253	3.4789	3.0987	2.5649	2.1418	1.2324	0.0501	0.0399	0.0053
2C-13_89	13.7935	4.4394	2.5896	5.1264	8.5523	8.0316	6.2381	5.8072	3.8041	0.2737	0.0485	0.0000
3C-3_87	8.9858	2.6405	1.6484	1.7117	4.2414	3.9919	2.1366	2.3603	1.0934	0.0000	0.0741	0.0022
2B-2_87	9.1125	2.7308	1.5403	1.7929	4.9042	4.7022	2.2497	2.7221	1.3096	0.0000	0.0304	0.0000
1A-11_89	32.8655	11.4086	0.1828	0.0657	22.6416	21.2890	0.0286	0.0000	0.0000	0.0000	0.1232	0.0943
3C-15_87	13.4641	4.6923	3.7531	4.5898	11.1423	11.3369	5.9621	6.9434	3.4671	0.0535	0.2218	0.0288
1B-1_87	17.5719	6.4459	0.1611	0.0524	13.1971	12.4793	0.0198	0.0000	0.0000	0.0000	0.0598	0.0548
1A-1_87	13.5682	4.6709	0.1406	0.0477	7.8500	6.8835	0.0098	0.0000	0.0045	0.0000	0.0489	0.0344
2A-13_89	14.1854	4.5623	2.9588	5.4740	8.5674	7.8744	6.4094	5.5626	3.3472	0.2786	0.0662	0.0143
3B-1_87	7.3997	2.1653	1.3604	1.4163	3.4277	3.2056	1.6991	1.8479	0.8063	0.0000	0.0583	0.0000

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1B-17_89	9.4974	6.1208	0.1364	0.1631	42.5755	53.4152	0.0635	0.0000	0.0000	0.0000	0.5090	0.4787
1A-6_89	23.4387	7.8853	0.1689	0.0595	14.2769	12.9037	0.0168	0.0000	0.0000	0.0000	0.0996	0.0730
3B-3_89	8.1898	2.4222	1.1906	2.0454	3.2694	3.0354	2.3391	1.9911	1.1242	0.0199	0.0531	0.0055
1C-14_89	33.4270	12.7004	0.2964	0.1282	29.9221	28.9050	0.0364	0.0000	0.0228	0.0000	0.1991	0.1785
3A-19_87	0.1483	0.1713	0.9982	3.3249	5.6518	10.0006	7.8772	15.5961	9.7339	0.3574	0.7364	0.2053
3C-5_89	8.7430	2.5994	1.2920	2.2285	3.5168	3.2978	2.5693	2.2064	1.2921	0.0470	0.0529	0.0042
1C-8_89	27.6732	9.3368	0.1944	0.0717	17.2410	15.7234	0.0240	0.0000	0.0000	0.0047	0.1109	0.0820
3B-11_87	12.8397	3.8559	2.4482	2.6217	6.5001	6.1739	3.2335	3.5246	1.7117	0.0056	0.1109	0.0052
2A-4_87	10.0002	3.0196	1.5505	1.9982	5.5855	5.4594	2.5656	3.1231	1.3662	0.0000	0.0182	0.0000
3C-10_89	11.0707	3.3681	1.7306	3.0411	4.9171	4.6819	3.5821	3.2291	2.0597	0.1092	0.0757	0.0096
4C-11_87	13.3643	4.0935	2.2760	1.1296	7.2174	5.9274	2.1656	0.5470	0.0896	0.0000	0.0322	0.0000
1C-3_89	20.0827	6.7236	0.1354	0.0447	12.0507	10.9135	0.0150	0.0000	0.0000	0.0000	0.0936	0.0654
3B-5_89	8.3367	2.4814	1.2091	2.1245	3.3957	3.1813	2.4527	2.0990	1.2411	0.0390	0.0534	0.0069
2C-12_89	11.7110	3.6221	2.1203	3.8066	6.2457	5.7353	4.5372	4.0766	2.6562	0.2154	0.0609	0.0127
3B-6_87	9.6497	2.8467	1.7814	1.8065	4.6180	4.3645	2.2901	2.5513	1.1908	0.0000	0.0768	0.0023
3A-3_89	8.3304	2.4840	1.2277	2.1289	3.3573	3.1401	2.4652	2.1321	1.2382	0.0284	0.0503	0.0066
3B-9_87	11.7286	3.4815	2.1344	2.2530	5.6940	5.3700	2.7621	3.0688	1.4955	0.0050	0.0898	0.0030
3A-15_87	13.7131	4.7147	3.6608	4.4159	10.6731	10.8123	5.6226	6.4692	3.2411	0.0472	0.2133	0.0330
4A-6_87	10.8831	3.2946	1.7959	0.8958	5.6358	4.6116	1.7031	0.4293	0.0653	0.0000	0.0375	0.0000

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1A-15_87	26.2080	11.0383	0.3838	0.1942	29.0939	28.6680	0.0548	0.0000	0.0066	0.0000	0.2091	0.1876
2B-13_89	14.6401	4.7525	3.0716	5.8146	9.3176	8.7371	6.9985	6.2836	3.9137	0.3289	0.0706	0.0191
1A-3_89	20.7761	7.0865	0.1530	0.0541	13.2592	12.1533	0.0165	0.0000	0.0000	0.0000	0.0941	0.0620
3C-10_87	11.1480	3.3198	2.0820	2.1983	5.5049	5.2077	2.7377	2.9751	1.4269	0.0046	0.0867	0.0026
2A-13_87	15.8768	5.1653	3.2811	4.0885	11.4657	11.6142	5.5575	7.2717	4.0312	0.0119	0.0699	0.0042
3C-2_89	7.5677	2.2442	1.0929	1.9668	3.0656	2.8847	2.2722	2.0233	1.2130	0.0124	0.0491	0.0020
4C-17_87	7.5405	3.8668	4.7058	3.7922	21.4014	22.6350	9.1188	3.3189	1.4908	0.0537	0.2444	0.1249
2A-19_87	0.0074	0.0325	0.4514	2.6526	4.7633	11.2980	9.0905	27.5539	21.6798	0.9016	0.5569	0.2438
1C-19_87	0.2985	0.3193	0.0102	0.0560	12.5300	28.7169	0.0499	0.0237	0.0000	0.0156	1.7773	1.7168
4C-7_87	11.5600	3.4962	1.8764	0.9363	5.9727	4.8755	1.7699	0.4542	0.0544	0.0000	0.0199	0.0000
1C-4_87	18.9982	6.6334	0.1698	0.0610	11.7467	10.4325	0.0178	0.0000	0.0000	0.0000	0.0635	0.0488
3A-14_89	16.3208	5.4123	3.3070	6.2061	9.7380	9.5666	7.5741	7.0251	4.3788	0.3620	0.1588	0.0527
2C-4_87	10.6048	3.1956	1.7450	2.0440	5.9110	5.7579	2.6580	3.2966	1.6539	0.0000	0.0398	0.0000
4C-4_87	10.3095	3.0985	1.6780	0.8377	5.2655	4.2677	1.5835	0.3695	0.0478	0.0000	0.0241	0.0000
1C-8_87	27.6667	9.8988	0.2270	0.0856	19.1765	17.7504	0.0293	0.0000	0.0000	0.0000	0.0768	0.0457
1B-12_89	32.8797	11.4166	0.2480	0.1063	22.2187	20.5050	0.0257	0.0000	0.0000	0.0000	0.1491	0.1156
3A-13_89	15.6251	5.0056	2.7507	5.0442	8.1949	8.0119	6.1018	5.6785	3.6856	0.3588	0.1182	0.0303
2B-3_87	9.7277	2.9332	1.7270	1.9008	5.2839	5.1002	2.4683	2.9213	1.4540	0.0000	0.0364	0.0020
3B-7_89	10.1810	3.0626	1.5000	2.6673	4.3106	4.0638	3.1377	2.7838	1.7242	0.0938	0.0596	0.0080

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1B-16_87	24.8304	11.0608	0.3915	0.2130	33.0972	21.0213	0.0550	0.0000	0.0186	0.0000	0.2304	0.2096
3A-16_89	11.4560	4.6563	4.0631	9.1340	13.6902	14.9890	12.4392	12.6353	8.3580	0.7115	0.2633	0.1013
3A-14_89	16.6672	5.5462	3.3750	6.3599	10.1297	10.0483	7.8263	7.2903	4.6873	0.4030	0.1522	0.0511
3A-15_87	13.6148	4.6790	3.6482	4.3998	10.5845	10.6875	5.6536	6.5214	3.2712	0.0458	0.2251	0.0283
4B-12_87	13.9562	4.3067	2.4227	1.2295	7.7241	6.3810	2.3566	0.6382	0.1027	0.0000	0.0308	0.0000
1B-8_87	25.9806	9.2606	0.2102	0.0608	17.5792	16.2636	0.0225	0.0000	0.0000	0.0000	0.0667	0.0392
3C-5_87	9.5599	2.8104	1.7439	1.8208	4.5150	4.2433	2.2091	2.4609	1.1569	0.0000	0.0698	0.0000
2C-4_87	10.4990	3.1817	1.6959	2.0642	5.9474	5.8279	2.7143	3.3729	1.6088	0.0000	0.0267	0.0000
3A-3_89	8.4775	2.5307	1.2314	2.1881	3.4534	3.2517	2.5143	2.2018	1.2395	0.0202	0.0500	0.0085
3A-6_89	9.6472	2.8950	1.4331	2.5198	4.0491	3.8235	2.9352	2.5927	1.6291	0.0645	0.0581	0.0098
2B-6_87	11.0651	3.3728	1.6622	2.1586	6.4532	6.4188	2.9127	3.6615	1.5359	0.0000	0.0178	0.0000
3A-5_89	8.6786	2.5966	1.2966	2.2838	3.5887	3.3729	2.6265	2.2977	1.3866	0.0275	0.0563	0.0080
3B-1_87	7.4060	2.1618	1.3420	1.3940	3.4349	3.1846	1.6831	1.8801	0.8110	0.0000	0.0528	0.0000
1B-12_87	30.7016	11.0673	0.3046	0.1528	21.1683	19.3111	0.0288	0.0000	0.0000	0.0000	0.1216	0.1151
1A-10_87	31.2716	11.3438	0.2521	0.0865	22.4678	20.9974	0.0303	0.0000	0.0000	0.0000	0.0924	0.0673
2C-1_87	7.9177	2.3630	1.1707	1.4774	4.2421	4.1050	1.8402	2.3017	0.8020	0.0000	0.0133	0.0000
2A-9_87	12.1721	3.6865	2.2121	2.3780	6.6729	6.3594	2.9523	3.4286	1.7294	0.0036	0.0574	0.0107
3B-16_87	7.2173	3.1343	3.5939	5.2723	11.9878	13.5384	7.4989	9.5103	4.9368	0.1646	0.3334	0.0695
1C-15_89	29.5369	11.9173	0.3017	0.1700	31.5791	19.9743	0.0410	0.0000	0.0000	0.0000	0.2512	0.2143

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1B-3_89	19.5123	6.5286	0.1443	0.0423	11.5819	10.4079	0.0131	0.0000	0.0000	0.0000	0.0818	0.0562
2B-1_87	7.5603	2.2591	1.1338	1.4497	4.0386	3.8888	1.8356	2.2805	0.9461	0.0000	0.0173	0.0000
3A-2_89	7.5071	2.2304	1.1046	1.9354	3.0330	2.8216	2.2413	1.9369	1.0615	0.0220	0.0490	0.0038
1C-17_87	9.9704	6.1818	0.2814	0.2343	36.7679	43.8202	0.0842	0.0000	0.0000	0.0000	0.4217	0.4003
1A-16_89	27.8048	11.7503	0.3013	0.1664	34.6507	35.3533	0.0447	0.0000	0.0000	0.0000	0.2702	0.2447
4B-2_87	9.6946	2.9198	1.5435	0.7672	4.9481	4.0210	1.4571	0.3581	0.0346	0.0000	0.0260	0.0000
1C-14_87	30.9222	12.2417	0.4141	0.1863	28.9344	27.7436	0.0483	0.0000	0.0000	0.0000	0.1917	0.1666
1C-12_89	34.7067	12.0785	0.2432	0.1062	24.1690	22.6004	0.0278	0.0000	0.0000	0.0000	0.1460	0.1205
4C-12_87	13.5753	4.1732	2.3716	1.1994	7.4390	6.1258	2.2650	0.6032	0.0869	0.0000	0.0321	0.0000
2C-11_89	9.9177	3.0315	1.7241	3.1004	5.1516	4.6982	3.6408	3.2551	2.0963	0.1852	0.0519	0.0115
1B-9_89	28.5362	9.7172	0.1983	0.0798	18.2498	16.7466	0.0239	0.0000	0.0000	0.0046	0.1196	0.0971
2C-9_89	8.2321	2.4661	1.4422	2.5200	3.8920	3.4855	2.9038	2.4561	1.4621	0.0796	0.0419	0.0035
3B-15_89	16.3650	5.8313	3.9092	7.7754	12.5221	12.7808	9.8845	9.5982	6.2968	0.5464	0.1891	0.0772
1B-3_87	16.2520	5.5921	0.1646	0.0598	9.4485	8.3423	0.0160	0.0000	0.0000	0.0000	0.0660	0.0434
4A-15_87	19.0251	6.6378	4.5822	2.5924	15.9774	10.0163	5.2837	1.6695	0.6180	0.0087	0.1129	0.0405
2A-6_89	8.7748	2.6422	1.4594	2.6529	4.2737	3.8433	3.1002	2.7283	1.6966	0.0888	0.0442	0.0066
1B-15_87	29.7153	12.0315	0.4030	0.2048	29.5128	17.6138	0.0444	0.0000	0.0209	0.0000	0.1952	0.1816
1C-8_89	27.6210	9.3575	0.1826	0.0747	17.4375	16.1125	0.0188	0.0000	0.0000	0.0000	0.1121	0.0813
2C-19_87	0.0460	0.0855	0.7723	3.5020	6.7081	13.9520	10.1665	25.7802	18.3119	0.7402	0.4649	0.1949

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1A-15_89	33.6845	13.0858	0.2963	0.1422	32.6061	31.9825	0.0391	0.0000	0.0000	0.0000	0.2087	0.1872
4A-8_87	11.6468	3.5301	1.9419	0.9596	6.1066	4.9999	1.8296	0.4930	0.0628	0.0000	0.0341	0.0037
2C-4_87	10.2535	3.0794	1.7359	2.0187	5.6730	5.5153	2.6024	3.2263	1.5839	0.0000	0.0420	0.0000
3A-5_87	9.3585	2.7604	1.6693	1.7392	4.4315	4.1792	2.1981	2.4525	1.1154	0.0047	0.0766	0.0000
1A-13_87	31.0498	11.6851	0.3868	0.1688	24.5811	22.9257	0.0403	0.0000	0.0000	0.0000	0.1558	0.1531
1A-3_89	20.3710	6.9288	0.1547	0.0572	12.7575	11.5666	0.0173	0.0000	0.0000	0.0000	0.0913	0.0639
4C-14_87	18.3092	6.0120	3.8597	2.0811	12.6912	10.8813	4.0723	1.2695	0.3392	0.0000	0.0816	0.0200
4B-8_87	11.9132	3.6041	1.9365	0.9798	6.2162	5.0926	1.8197	0.5040	0.0766	0.0000	0.0360	0.0000
1C-1_87	13.2046	4.5561	0.1372	0.0546	7.6761	6.7293	0.0116	0.0000	0.0062	0.0000	0.0509	0.0336
3B-11_87	12.8652	3.8699	2.4264	2.6240	6.5181	6.1916	3.1742	3.5254	1.7100	0.0096	0.0947	0.0057
3C-14_87	14.3496	4.6466	3.3300	3.8095	9.3172	9.1837	4.7359	5.3578	2.6283	0.0233	0.1741	0.0161
3B-15_89	16.2204	5.7553	3.8661	7.7282	12.3186	12.5760	9.7587	9.4033	6.1127	0.5201	0.1992	0.0684
2B-12_87	14.8111	4.6095	2.7877	3.2911	9.2953	9.2312	4.3650	5.5457	2.9588	0.0103	0.0624	0.0032
2A-14_87	16.4079	5.4747	3.7269	4.5787	12.8797	13.2166	6.1321	7.9550	4.2669	0.0214	0.0933	0.0184
1B-16_89	17.6871	8.9367	0.2755	0.1985	38.2571	42.9160	0.0608	0.0000	0.0099	0.0000	0.3734	0.3383
3C-15_87	13.3946	4.6691	3.7977	4.5929	11.0709	11.3827	5.9821	6.9095	3.4739	0.0741	0.2312	0.0324
1B-9_89	28.4696	9.6732	0.2208	0.0912	17.9243	16.2868	0.0199	0.0000	0.0000	0.0000	0.1209	0.0920
2B-18_89	0.0255	0.0449	0.7822	5.0496	3.8425	7.7971	13.4813	24.1960	18.9809	1.3941	0.5213	0.2563
2A-5_89	8.1684	2.4402	1.4073	2.4708	3.8933	3.5006	2.8920	2.5193	1.5389	0.0518	0.0372	0.0096

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2A-2_89	7.2161	2.1606	1.1452	2.1421	3.4154	3.0788	2.5273	2.2043	1.3027	0.0510	0.0288	0.0016
2B-10_87	13.1863	4.0231	2.4661	2.6556	7.4196	7.1104	3.3187	3.8959	1.9273	0.0080	0.0603	0.0021
1C-2_89	19.9088	6.6633	0.1401	0.0395	11.8959	10.7714	0.0136	0.0000	0.0000	0.0000	0.0809	0.0503
4A-17_87	8.0341	3.9889	4.7327	3.7001	20.3924	21.2060	8.7104	3.1850	1.5010	0.0423	0.2398	0.1226
3A-8_89	9.4978	2.8666	1.4230	2.5299	4.1276	3.9121	3.0119	2.6805	1.6535	0.0820	0.0590	0.0069
1A-18_89	12.9109	7.2722	0.2235	0.2078	38.7027	45.5524	0.0604	0.0000	0.0000	0.0000	0.4489	0.4005
3B-9_89	10.9714	3.3044	1.6560	2.9442	4.7014	4.4519	3.4312	3.0624	1.9421	0.1322	0.0637	0.0097
2B-5_87	10.4207	3.1266	1.6981	1.9675	5.7563	5.5819	2.5227	3.1610	1.5298	0.0000	0.0390	0.0000
3C-16_89	12.8652	4.8826	3.9587	8.0796	11.8851	12.4426	10.3335	9.7142	5.7956	0.4364	0.2325	0.0877
1C-11_89	31.7743	10.8911	0.2398	0.0930	20.5752	18.8226	0.0293	0.0000	0.0284	0.0000	0.1441	0.1065
4B-3_87	9.8199	2.9545	1.6134	0.8018	5.0005	4.0451	1.5152	0.3748	0.0367	0.0000	0.0219	0.0000
3C-8_87	10.4474	3.0983	1.9402	2.0059	5.0583	4.7723	2.4964	2.7659	1.3137	0.0000	0.0811	0.0021
4B-14_87	10.1507	4.6795	4.7336	3.4779	20.3267	20.5414	8.1212	2.9344	1.3451	0.0268	0.2106	0.1069
3C-5_89	8.4730	2.5111	1.2670	2.1405	3.3418	3.0977	2.4164	2.0412	1.1406	0.0336	0.0551	0.0054
3A-12_87	12.5965	3.7888	2.4201	2.5778	6.4515	6.1426	3.1940	3.4921	1.6657	0.0084	0.0891	0.0034
2A-5_87	9.8209	2.9655	1.6489	1.9487	5.4704	5.3100	2.6325	3.1234	1.5518	0.0000	0.0363	0.0000
3B-2_89	8.0842	2.3923	1.1733	2.0612	3.2499	3.0413	2.3853	2.0715	1.1828	0.0250	0.0404	0.0000
3A-4_87	8.9133	2.6240	1.6241	1.6488	4.1969	3.9456	2.1226	2.3070	1.0439	0.0000	0.0728	0.0021
3C-18_89	2.5047	1.5251	2.9160	9.0697	11.3930	15.1289	14.8940	17.6315	11.6017	0.8583	0.4422	0.2012

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
3B-7_87	10.6616	3.1449	1.9583	2.0017	5.0898	4.7849	2.4842	2.7004	1.2857	0.0000	0.0835	0.0048
2B-17_89	1.1717	0.8402	2.5601	9.1696	10.3067	14.0567	16.0661	20.1880	13.8669	1.1037	0.3262	0.1757
2B-2_87	9.3785	2.8437	1.3736	1.8538	5.2436	5.1288	2.3414	3.0487	1.2445	0.0000	0.0221	0.0000
1A-19_89	4.6941	3.5673	0.1529	0.2065	36.0646	49.0714	0.0732	0.0455	0.0000	0.0030	0.6957	0.6376
2C-18_89	0.0163	0.0308	0.5849	4.1580	3.0681	6.5407	12.0662	24.0216	20.2902	1.5249	0.5824	0.2992
1B-18_89	1.6321	0.9549	0.0244	0.0224	8.0134	18.9464	0.0205	0.0437	0.0149	0.0162	3.7643	3.7341
3B-4_89	8.6393	2.5605	1.2728	2.1799	3.4325	3.2053	2.4915	2.1390	1.1820	0.0296	0.0459	0.0065
3B-18_87	0.0416	0.0538	0.4556	2.1515	3.3393	7.2179	6.6002	16.7276	11.4008	0.4120	0.8881	0.2492
2A-1_89	6.8330	2.0464	1.0732	2.0573	3.2793	2.9657	2.4509	2.2305	1.3580	0.0413	0.0242	0.0000
2B-8_87	13.1005	4.0274	2.1561	2.6143	7.8567	7.7829	3.3980	4.2871	2.2233	0.0000	0.0373	0.0000
2B-7_89	8.8157	2.6343	1.5078	2.6180	4.1780	3.7409	3.0096	2.5443	1.4767	0.0664	0.0432	0.0047
4A-7_87	11.2310	3.3982	1.8633	0.9249	5.8264	4.7675	1.7660	0.4560	0.0769	0.0000	0.0315	0.0000
3C-6_89	9.1581	2.7497	1.3703	2.4464	3.8942	3.6987	2.8611	2.5860	1.5882	0.0515	0.0596	0.0084
3A-18_89	1.1646	0.8407	2.3652	8.3752	9.3217	13.3838	14.8788	19.1711	13.2709	1.0206	0.5102	0.2067
1B-16_87	23.8310	10.5818	0.4045	0.2232	31.3441	31.7351	0.0565	0.0000	0.0122	0.0000	0.2316	0.2140
2C-13_87	15.9187	5.1357	3.2015	3.8165	11.0974	11.1667	5.0616	6.3212	3.3435	0.0000	0.0888	0.0114
3A-9_89	10.8846	3.3020	1.6416	2.9461	4.7721	4.5438	3.4412	3.1200	1.9766	0.1325	0.0687	0.0088
4B-5_87	10.3634	3.1251	1.7035	0.8370	5.3254	4.3145	1.5995	0.3976	0.0631	0.0000	0.0345	0.0000
2C-5_89	8.0699	2.4098	1.3625	2.4019	3.8071	3.4145	2.7777	2.4029	1.3986	0.0375	0.0339	0.0062

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
3B-6_89	9.3050	2.7836	1.3719	2.4598	3.8975	3.6736	2.8522	2.5522	1.6166	0.0966	0.0606	0.0083
2C-2_89	5.8720	1.7487	0.9771	1.7129	2.6856	2.3912	1.9839	1.6530	0.9311	0.0230	0.0229	0.0000
2B-10_89	9.4499	2.8640	1.6846	2.9872	4.6984	4.2474	3.4619	2.9544	1.8119	0.1297	0.0544	0.0095
1A-1_87	13.5450	4.6785	0.1364	0.0467	7.8760	6.9097	0.0119	0.0000	0.0000	0.0000	0.0522	0.0346
3A-7_87	10.2473	3.0200	1.8849	1.9833	4.9142	4.6424	2.4423	2.7251	1.2808	0.0047	0.0915	0.0020
1C-7_89	25.9083	8.8113	0.1667	0.0761	16.4701	15.3574	0.0160	0.0000	0.0000	0.0000	0.1041	0.0780
1A-8_89	27.4690	9.3259	0.1634	0.0501	17.4243	16.1449	0.0169	0.0000	0.0000	0.0000	0.0851	0.0759
4C-8_87	12.0486	3.6448	1.9558	0.9819	6.2717	5.1212	1.8459	0.5079	0.0616	0.0000	0.0308	0.0000
3A-8_87	11.1236	3.2902	2.0470	2.1108	5.3510	5.0305	2.5838	2.8719	1.3804	0.0000	0.0773	0.0022
1C-11_89	30.8497	10.5881	0.2300	0.1010	19.8789	18.1423	0.0192	0.0000	0.0000	0.0000	0.1396	0.1036
2C-12_89	11.9209	3.6833	2.1523	3.8970	6.3836	5.8574	4.5876	4.1103	2.6102	0.2385	0.0640	0.0165
2B-3_89	7.4273	2.2169	1.2466	2.1609	3.4705	3.1116	2.5159	2.1612	1.2816	0.0748	0.0325	0.0059
3B-13_89	15.7884	5.0351	2.8008	5.0931	8.2717	8.0208	6.1180	5.6361	3.6523	0.3337	0.1164	0.0409
1B-4_87	17.2614	5.9438	0.1755	0.0618	10.0574	8.9017	0.0150	0.0000	0.0000	0.0000	0.0776	0.0448
1B-15_87	30.6360	12.4517	0.3946	0.2048	30.9122	30.1417	0.0494	0.0000	0.0000	0.0000	0.1937	0.1762
3A-7_89	10.0441	3.0074	1.5078	2.6189	4.2159	3.9693	3.0653	2.6682	1.6144	0.0775	0.0662	0.0076
1C-19_87	0.3013	0.3148	0.0133	0.0641	12.5613	28.9676	0.0554	0.0271	0.0053	0.0073	1.7684	1.7831
1B-3_87	16.3155	5.6154	0.1617	0.0582	9.4789	8.1735	0.0122	0.0000	0.0087	0.0000	0.0677	0.0487
2B-3_87	9.4300	2.8268	1.6377	1.9327	5.1095	4.8809	2.4854	3.0042	1.4965	0.0000	0.0351	0.0000

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
3A-6_87	9.8600	2.9075	1.8011	1.9007	4.6941	4.4190	2.3314	2.5543	1.2041	0.0000	0.0735	0.0023
2A-8_87	11.8077	3.5728	2.0593	2.3524	6.6030	6.4226	2.9962	3.6973	1.8863	0.0000	0.0458	0.0000
1B-9_89	28.9914	9.8757	0.2098	0.0923	18.5120	17.0186	0.0203	0.0000	0.0000	0.0000	0.1307	0.0865
1A-13_87	29.6884	11.0716	0.4132	0.1701	23.1301	21.5997	0.0396	0.0000	0.0045	0.0000	0.1591	0.1508
3B-6_87	9.5612	2.8197	1.7799	1.8469	4.5814	4.3241	2.2650	2.5544	1.2070	0.0000	0.0829	0.0026
3C-2_87	8.2302	2.4135	1.5181	1.5408	3.8820	3.6291	1.9692	2.1856	0.9908	0.0000	0.0673	0.0000
2A-8_89	8.1906	2.4492	1.4331	2.4304	3.8029	3.3846	2.7719	2.3010	1.2885	0.0363	0.0427	0.0048
1A-8_89	26.3285	8.8943	0.1734	0.0605	16.3013	14.9292	0.0156	0.0000	0.0000	0.0000	0.1032	0.0731
2B-12_89	11.6626	3.6285	2.1101	3.8890	6.4875	5.9830	4.6312	4.1528	2.6801	0.2644	0.0555	0.0171
4C-12_87	13.5635	4.1681	2.3579	1.1818	7.4506	6.1257	2.2589	0.6031	0.1052	0.0000	0.0360	0.0000
3C-1_89	7.4675	2.2099	1.0924	1.8630	2.9356	2.7236	2.1323	1.7970	0.9282	0.0082	0.0467	0.0000
3C-3_89	8.2687	2.4401	1.2304	2.0736	3.2488	3.0088	2.3453	1.9805	1.0285	0.0152	0.0542	0.0018
2B-1_87	7.5766	2.2602	1.2166	1.4303	4.0316	3.8832	1.8966	2.2394	0.8909	0.0000	0.0153	0.0000
4B-3_87	9.7899	2.9410	1.5907	0.7937	4.9860	4.0307	1.4917	0.3692	0.0515	0.0000	0.0280	0.0000
2C-14_89	14.3858	4.8199	3.3687	6.4123	9.9516	9.2834	7.6748	6.7515	4.0066	0.3286	0.0864	0.0240
1A-10_89	27.7087	9.4396	0.2316	0.0877	17.5546	15.8526	0.0249	0.0000	0.0000	0.0000	0.1140	0.0900
1C-3_87	16.2188	5.5818	0.1664	0.0651	9.4160	8.1202	0.0144	0.0000	0.0000	0.0000	0.0657	0.0394
2B-15_89	12.2418	4.5647	3.9180	8.1524	12.2769	12.1910	10.3701	9.6264	5.7963	0.4653	0.1266	0.0462
3C-13_89	14.9919	4.7280	2.6766	4.7856	7.5427	7.2588	5.6816	5.1008	3.0619	0.2667	0.1139	0.0353

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1C-1_87	13.2191	4.5628	0.1388	0.0516	7.6786	6.7278	0.0102	0.0000	0.0000	0.0000	0.0462	0.0326
2A-16_89	7.9831	3.5089	4.0814	9.5371	13.5341	14.2896	12.8890	12.5377	7.6957	0.6050	0.1768	0.0686
2B-11_89	10.3058	3.1522	1.9126	3.4341	5.3081	4.8011	4.0144	3.4733	2.1407	0.1729	0.0598	0.0145
1A-11_89	30.2015	10.2594	0.2336	0.1033	19.0898	17.4168	0.0243	0.0000	0.0338	0.0000	0.1399	0.1110
2A-11_87	13.3159	4.1025	2.5364	2.8350	7.8825	7.6852	3.5858	4.3620	2.2269	0.0153	0.0613	0.0047
1C-18_89	1.2253	1.3624	0.0580	0.1447	29.9573	50.1251	0.0768	0.0390	0.0000	0.0048	1.0835	1.0181
1B-8_89	26.5816	8.9986	0.1862	0.0746	16.6532	15.2232	0.0164	0.0000	0.0083	0.0000	0.1085	0.0827
2A-7_87	11.4274	3.4784	1.9923	2.2371	6.3687	6.1539	2.8197	3.3872	1.7252	0.0044	0.0505	0.0021
1A-18_87	3.7365	2.8143	0.1771	0.1936	24.1818	31.5340	0.0670	0.0188	0.0000	0.0000	0.5221	0.5136
1A-16_87	21.7556	10.4135	0.3749	0.2414	36.5592	38.6736	0.0650	0.0000	0.0000	0.0000	0.2613	0.2547
1A-13_87	31.5078	11.8443	0.3859	0.1611	25.0486	23.4510	0.0407	0.0000	0.0000	0.0000	0.1598	0.1557
4B-14_87	10.2197	4.7138	4.7385	3.4843	20.4504	16.5285	8.1474	2.9529	1.2959	0.0284	0.2152	0.0980
2C-11_87	13.8665	4.2840	2.5214	2.9301	8.3763	8.2630	3.8597	4.8510	2.5023	0.0000	0.0524	0.0000
1A-14_87	30.4256	11.9484	0.4037	0.1801	27.6611	26.3479	0.0421	0.0034	0.0000	0.0000	0.1767	0.1521
2B-5_89	7.7825	2.3248	1.5195	2.4266	3.7084	3.3388	2.7711	2.3689	1.2486	0.0059	0.0424	0.0071
3A-9_87	11.2143	3.3233	2.0636	2.1753	5.4429	5.1402	2.6240	2.9650	1.4056	0.0048	0.0914	0.0030
3B-8_89	10.2418	3.0826	1.5409	2.7005	4.3479	4.1051	3.1566	2.7926	1.7049	0.0793	0.0620	0.0113
2A-6_89	8.7752	2.6352	1.4777	2.6489	4.2422	3.8201	3.0924	2.7236	1.6880	0.0732	0.0470	0.0091
4A-8_87	11.6558	3.5342	1.9135	0.9624	6.1058	5.0091	1.8439	0.4925	0.0719	0.0000	0.0329	0.0036

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1B-2_89	18.2725	6.0656	0.1373	0.0534	10.5859	9.5195	0.0123	0.0000	0.0000	0.0000	0.0780	0.0523
3B-10_89	11.5814	3.5302	1.7322	3.1726	5.1781	4.9688	3.7225	3.4427	2.2154	0.0884	0.0615	0.0082
2A-16_89	7.6998	3.3813	3.9881	9.2298	12.8026	13.6960	12.4204	11.9405	7.1222	0.5425	0.1694	0.0751
3B-13_87	14.8956	4.7576	3.2767	3.6974	9.0478	8.8196	4.4851	5.0257	2.5222	0.0102	0.1627	0.0187
2C-3_89	7.8620	2.3609	1.1647	2.3091	3.8820	3.5493	2.7574	2.4523	1.1593	0.0000	0.0184	0.0000
4A-13_87	17.5085	5.5756	3.3618	1.7008	10.9167	9.2373	3.4023	1.0360	0.2838	0.0000	0.0619	0.0107
3C-7_87	10.7607	3.1836	1.9659	2.0491	5.1669	4.8635	2.5029	2.7473	1.3226	0.0046	0.0819	0.0024
2C-9_89	8.3114	2.5027	1.4334	2.5768	4.0026	3.5886	2.9950	2.5779	1.5453	0.0894	0.0469	0.0036
3B-16_89	9.8818	4.2139	3.9917	9.2879	13.6519	15.1846	12.8629	13.3334	8.9819	0.7578	0.2984	0.1307
3A-16_87	11.1435	4.2364	3.9154	5.1682	12.1145	12.9174	6.8758	8.3021	4.2366	0.1286	0.2829	0.0604
3C-7_87	10.8160	3.1867	1.9568	2.0410	5.1777	4.8737	2.5021	2.7436	1.2784	0.0000	0.0870	0.0050
3B-2_87	8.1848	2.4089	1.4793	1.5489	3.8312	3.5955	1.9111	2.1021	0.9368	0.0000	0.0716	0.0019
2C-16_87	10.5093	4.2352	3.9617	5.7432	14.8964	16.3348	8.2960	10.9708	6.0868	0.2620	0.1754	0.0569
2A-6_87	11.2107	3.4279	1.8951	2.1741	6.5304	6.2830	2.8093	3.4251	1.8372	0.0145	0.0513	0.0019
1B-6_89	23.2289	7.7323	0.1797	0.0794	13.6691	12.3058	0.0138	0.0000	0.0000	0.0000	0.1018	0.0730
1C-10_87	29.9563	10.7688	0.2594	0.1124	20.7368	19.0568	0.0276	0.0000	0.0178	0.0000	0.1053	0.0792
3A-10_87	11.4506	3.4151	2.1206	2.2487	5.6332	5.3363	2.7498	3.0408	1.4558	0.0049	0.0953	0.0027
3B-1_89	7.8917	2.3496	1.1767	2.0311	3.1824	2.9705	2.3329	1.9944	1.1862	0.0371	0.0566	0.0064
2B-8_89	9.0571	2.7221	1.5737	2.8265	4.3583	3.9232	3.2844	2.8361	1.7130	0.0732	0.0484	0.0059

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
4C-16_87	16.1374	6.2594	5.1239	3.1842	18.9649	18.1697	6.7706	2.2226	0.8644	0.0123	0.1457	0.0547
1B-12_87	31.6606	11.4834	0.3137	0.1334	22.4036	20.5650	0.0322	0.0000	0.0000	0.0000	0.1145	0.0975
2A-5_89	8.1601	2.4420	1.4060	2.4932	3.9262	3.5459	2.9233	2.5865	1.4821	0.0250	0.0283	0.0020
4A-11_87	13.8049	4.2556	2.3890	1.2050	7.6303	6.3220	2.3150	0.6881	0.1527	0.0000	0.0376	0.0043
2C-17_87	4.8254	2.5216	3.4749	6.2347	16.2896	20.3405	10.2240	15.7875	9.1364	0.4056	0.2344	0.0828
3B-15_89	15.9859	5.6760	3.8343	7.5978	12.0158	12.2430	9.5760	9.0355	5.6950	0.4615	0.1937	0.0687
3C-5_89	8.7969	2.6334	1.2961	2.2901	3.6121	3.3940	2.6629	2.3043	1.3627	0.0478	0.0592	0.0000
4C-18_87	1.5591	1.2178	2.9116	3.6385	17.5959	23.3672	10.8017	5.1109	2.5105	0.2011	0.4154	0.2231
2B-9_89	8.8156	2.6493	1.5586	2.7476	4.2160	3.7813	3.1612	2.6758	1.5695	0.0879	0.0478	0.0095
1B-1_87	17.0982	6.2302	0.1467	0.0404	12.6257	11.9346	0.0188	0.0000	0.0000	0.0000	0.0508	0.0400
2A-1_89	6.9576	2.0946	1.0595	2.1058	3.4239	3.1179	2.5335	2.3452	1.3422	0.0247	0.0316	0.0000
3B-7_87	10.5716	3.1231	1.9581	2.0187	5.0536	4.7474	2.4762	2.7270	1.2787	0.0047	0.0894	0.0051
2A-4_89	7.6318	2.2842	1.2709	2.2888	3.5974	3.2222	2.6509	2.3029	1.3787	0.0658	0.0382	0.0042
3A-14_87	13.9027	4.4802	3.2484	3.7074	8.9484	5.3225	4.6576	5.2258	2.6000	0.0203	0.1731	0.0188
2C-1_89	6.7934	2.0245	1.0760	2.0218	3.2426	2.9198	2.4066	2.1945	1.2770	0.0205	0.0264	0.0000
3B-8_87	10.9361	3.2436	2.0159	2.1120	5.3114	5.0231	2.6150	2.9240	1.3793	0.0047	0.0941	0.0027
3C-16_87	8.4493	3.4941	3.6528	5.1915	11.9074	13.4156	7.1975	9.0706	4.6501	0.1815	0.3333	0.0718
2A-5_87	10.2853	3.1067	1.7241	2.0125	5.8161	5.6916	2.6452	3.2193	1.6152	0.0000	0.0451	0.0000
4A-18_87	0.3421	0.3970	1.6212	2.9063	12.9433	21.3295	10.4172	6.4551	3.5897	0.3147	0.6330	0.3579

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
3C-8_87	10.5374	3.1218	1.8996	2.0142	5.1104	4.8264	2.5119	2.7813	1.2983	0.0000	0.0783	0.0000
2C-2_89	7.0786	2.1148	1.1250	2.0618	3.3581	3.0223	2.4239	2.1655	1.2472	0.0351	0.0212	0.0000
3B-14_89	16.4957	5.4795	3.4173	6.3102	9.8653	9.6843	7.6965	7.0388	4.4360	0.3692	0.1636	0.0543
1C-16_87	20.1333	10.0308	0.3534	0.2414	37.7669	40.6047	0.0657	0.0000	0.0000	0.0000	0.2887	0.2545
1A-9_87	28.0852	10.0743	0.2554	0.0955	19.2933	17.6351	0.0262	0.0000	0.0076	0.0000	0.0958	0.0781
3B-9_89	10.9320	3.2955	1.6483	2.9949	4.7334	4.4748	3.4648	3.1349	2.0015	0.1424	0.0658	0.0115
4C-6_87	10.8271	3.2697	1.7733	0.8732	5.5897	4.5394	1.6664	0.4089	0.0606	0.0000	0.0335	0.0000
1C-3_87	16.1754	5.5610	0.1668	0.0597	9.3659	8.0804	0.0142	0.0000	0.0039	0.0000	0.0703	0.0452
2C-2_87	8.6628	2.6080	1.3785	1.6940	4.6483	4.5265	2.1486	2.7072	1.1562	0.0000	0.0214	0.0000
2C-17_89	1.6184	1.0545	2.6832	8.7785	10.3610	13.4776	14.6644	17.3952	11.4873	0.8663	0.3077	0.1371
2B-16_89	4.8993	2.3834	3.4710	8.7206	11.4332	12.8551	12.2341	12.1423	6.9727	0.4804	0.2185	0.0961
1B-11_87	30.6528	11.0206	0.2942	0.1237	21.1189	19.2239	0.0307	0.0000	0.0000	0.0000	0.1048	0.0939
1C-5_89	22.1680	7.4742	0.1554	0.0625	13.5522	12.2853	0.0155	0.0000	0.0062	0.0000	0.0940	0.0598
1C-9_89	28.3870	9.7637	0.1584	0.0589	18.8925	17.8875	0.0106	0.0000	0.0000	0.0000	0.0942	0.0590
3C-15_89	16.6355	5.6865	3.6966	7.0940	11.0080	11.0642	8.8065	8.3054	5.3233	0.4660	0.1702	0.0574
4B-10_87	12.8353	3.9219	2.1748	1.0861	6.8751	5.6600	2.0772	0.5624	0.0896	0.0000	0.0384	0.0041
4A-3_87	9.7408	2.9277	1.5984	0.7857	4.9600	4.0084	1.4925	0.3569	0.0431	0.0000	0.0299	0.0000
2B-18_89	0.0261	0.0445	0.7837	5.1523	3.8661	7.8692	13.8483	25.0903	20.0463	1.5069	0.5194	0.2630
3A-14_87	13.7125	4.4599	3.2352	3.6656	8.8994	8.7825	4.6119	5.2049	2.5850	0.0252	0.1728	0.0209

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2C-9_87	12.4950	3.7835	2.2516	2.4870	6.9776	6.7400	3.1880	3.7295	1.8642	0.0044	0.0540	0.0022
3B-8_89	10.4705	3.1495	1.5683	2.8224	4.5181	4.2754	3.2786	2.9578	1.9180	0.1194	0.0606	0.0105
2C-2_89	7.0347	2.0993	1.1673	2.1501	3.3574	3.0159	2.5082	2.2623	1.4196	0.0582	0.0314	0.0033
3C-7_87	10.6711	3.1524	1.9645	2.0918	5.1219	4.8220	2.5299	2.7736	1.3229	0.0049	0.0900	0.0026
1B-19_87	3.8292	3.2999	0.1340	0.1928	39.0841	55.2755	0.1054	0.0000	0.0000	0.0000	0.6516	0.6168
1B-7_89	26.5396	9.0055	0.1748	0.0737	16.7629	15.3977	0.0219	0.0000	0.0119	0.0000	0.1035	0.0740
2B-5_89	7.7652	2.3231	1.3219	2.4084	3.7226	3.3383	2.8169	2.4814	1.5365	0.0757	0.0405	0.0072
3C-19_89	0.1096	0.1348	1.1417	6.1574	5.5024	10.2679	14.6579	23.8945	17.9121	1.3305	0.7020	0.2929
4C-11_87	13.2658	4.0672	2.3183	1.1182	7.1637	5.8867	2.1758	0.5401	0.0826	0.0000	0.0219	0.0000
3C-1_87	7.2293	2.1155	1.2911	1.3574	3.3488	3.1021	1.6636	1.8590	0.7660	0.0000	0.0549	0.0000
2C-9_87	12.2207	3.6985	2.2605	2.4683	6.7940	6.5423	3.1166	3.6487	1.8408	0.0075	0.0605	0.0072
2A-17_87	4.3039	2.2707	3.2228	5.9964	14.5745	18.2452	9.7950	14.9987	8.7345	0.3795	0.2362	0.0825
4C-9_87	12.6017	3.8358	2.1529	1.0325	6.6021	5.3829	1.9911	0.5619	0.1000	0.0000	0.0258	0.0000
4B-5_87	10.4189	3.1378	1.7048	0.8367	5.3498	4.3392	1.5878	0.3946	0.0492	0.0000	0.0320	0.0000
3C-7_89	9.5697	2.8710	1.4538	2.5161	4.0328	3.8032	2.9357	2.6154	1.6696	0.1105	0.0593	0.0089
2B-6_89	8.5715	2.5856	1.4531	2.5931	4.1779	3.7734	3.0159	2.6760	1.6498	0.0468	0.0451	0.0019
3C-9_87	10.5897	3.1330	1.9804	2.0656	5.1574	4.8873	2.5544	2.8405	1.3512	0.0035	0.0812	0.0025
4B-14_87	10.1919	4.6998	4.7428	3.5142	20.4545	20.6753	8.1311	2.9409	1.2483	0.0243	0.2141	0.0987
1A-2_89	18.6655	6.2406	0.1221	0.0428	11.0265	9.9463	0.0116	0.0000	0.0000	0.0000	0.0620	0.0462

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2C-5_89	8.0310	2.3954	1.3620	2.4339	3.7984	3.4049	2.8552	2.4686	1.5138	0.0567	0.0426	0.0066
1A-13_89	35.9123	12.9602	0.2561	0.0929	27.6312	26.3298	0.0253	0.0000	0.0000	0.0000	0.1794	0.1367
1B-5_87	20.5228	7.2217	0.1956	0.0775	13.0585	11.7410	0.0197	0.0000	0.0052	0.0000	0.0775	0.0644
4B-12_87	14.0005	4.3105	2.4292	1.2244	7.7430	6.3913	2.3355	0.6505	0.1130	0.0000	0.0379	0.0022
4A-6_87	10.8776	3.2841	1.7871	0.8865	5.6230	4.6108	1.6781	0.4342	0.0689	0.0000	0.0324	0.0000
2B-5_87	10.4929	3.2051	1.3937	2.0674	6.1684	6.1148	2.5524	3.4311	1.3599	0.0000	0.0242	0.0000
1C-7_87	23.6048	8.3115	0.2230	0.0852	15.0579	13.5322	0.0215	0.0000	0.0062	0.0000	0.0750	0.0674
2B-13_89	13.9376	4.4974	3.0521	5.5672	8.5295	7.8887	6.6051	5.7854	3.4258	0.2598	0.0716	0.0196
3C-13_89	15.4197	4.8819	2.7010	4.9346	7.9217	7.6824	5.9229	5.3808	3.3925	0.2975	0.1163	0.0391
3A-2_87	8.4284	2.4722	1.5722	1.6216	3.9527	3.7134	1.9942	2.1884	0.9703	0.0000	0.0679	0.0000
1B-7_87	24.8124	8.8201	0.2056	0.0448	16.5896	15.2892	0.0208	0.0000	0.0000	0.0000	0.0534	0.0389
3C-6_87	10.1002	2.9817	1.8768	1.9152	4.8097	4.5266	2.3501	2.5931	1.2269	0.0000	0.0785	0.0042
3C-19_89	0.1097	0.1373	1.1380	6.2038	5.6562	10.6118	14.8805	24.4944	18.6564	1.4156	0.7082	0.3017
3A-8_87	10.8870	3.2273	2.0534	2.1229	5.2430	4.9376	2.5662	2.7959	1.4063	0.0067	0.0952	0.0066
3A-8_89	9.2404	2.7836	1.3887	2.4696	3.9273	3.7089	2.8590	2.5327	1.5131	0.0685	0.0548	0.0057
1B-5_89	22.8857	7.7090	0.1594	0.0621	14.0380	12.7833	0.0163	0.0000	0.0000	0.0000	0.0986	0.0629
2A-13_89	14.4273	4.6576	3.0389	5.5540	8.8440	8.1942	6.6202	5.7632	3.5022	0.3078	0.0689	0.0158
1B-10_89	31.1185	10.6496	0.2171	0.0907	19.9929	18.3503	0.0240	0.0000	0.0000	0.0000	0.1166	0.1014
3A-16_87	11.2070	4.2525	3.9426	5.1508	12.1927	12.9975	6.8681	8.3307	4.2399	0.1186	0.2758	0.0538

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
3C-2_89	7.5288	2.2349	1.0986	1.9140	3.0263	2.8339	2.2166	1.9303	1.1218	0.0260	0.0434	0.0000
2A-14_89	16.3671	5.6520	3.8238	7.6747	12.9841	12.6868	9.6120	9.0536	5.9298	0.5497	0.0869	0.0237
2A-4_87	9.6572	2.8964	1.5672	1.8886	5.2309	5.0679	2.3891	2.9810	1.2306	0.0000	0.0263	0.0000
2B-19_87	0.0000	0.0000	0.1007	1.3726	1.9810	6.4471	7.1214	30.0996	27.6239	1.1616	0.7247	0.3299
3B-11_89	12.8945	3.9343	2.0011	3.5629	5.8572	5.6113	4.1892	3.8532	2.5133	0.1287	0.0748	0.0113
3A-18_89	1.1823	0.8465	2.3575	8.3905	9.3749	13.4532	14.8449	19.0091	13.0101	0.9843	0.5016	0.2104
4C-2_87	9.5338	2.8671	1.5072	0.7549	4.8451	3.9207	1.4059	0.3391	0.0443	0.0000	0.0288	0.0000
4C-17_87	7.5283	3.8705	4.7608	3.8179	21.3904	22.6038	9.1726	3.3297	1.5002	0.0570	0.2415	0.1145
1C-3_89	19.7008	6.5716	0.1359	0.0464	11.6859	10.5295	0.0140	0.0025	0.0127	0.0000	0.0829	0.0531
4C-6_87	10.9112	3.2905	1.7736	0.8829	5.6374	4.5662	1.6733	0.4132	0.0550	0.0000	0.0312	0.0000
4B-8_87	11.8415	3.5896	1.9427	0.9717	6.1802	5.0612	1.8264	0.4741	0.0549	0.0000	0.0331	0.0022
3B-16_89	9.7494	4.1662	4.0818	9.2631	13.3410	14.7630	12.6741	13.1018	8.6092	0.7066	0.2920	0.1024
2C-7_87	11.1604	3.3564	1.9174	2.2369	6.2153	6.0497	2.8416	3.4831	1.7719	0.0000	0.0330	0.0000
3C-14_87	14.3159	4.6716	3.2806	3.8460	9.3722	9.2223	4.7902	5.3735	2.6628	0.0162	0.1732	0.0171
1C-17_89	10.8376	6.8242	0.1540	0.1605	45.6024	57.1436	0.0639	0.0000	0.0000	0.0000	0.5118	0.4825
4A-5_87	10.3960	3.1265	1.6974	0.8356	5.3165	4.3482	1.5936	0.3955	0.0517	0.0000	0.0283	0.0020
3C-18_87	0.3868	0.3409	1.2483	3.6761	6.8247	11.0763	8.0745	14.9371	9.0155	0.3196	0.6752	0.1812
4A-12_87	14.5155	4.4860	2.5566	1.2954	8.1252	6.7363	2.5057	0.7393	0.1280	0.0000	0.0449	0.0024
1B-15_87	32.1451	13.1265	0.3704	0.2071	33.3274	32.7103	0.0513	0.0000	0.0134	0.0000	0.1838	0.1747

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
3B-9_87	11.7519	3.4861	2.1933	2.2845	5.7004	5.3607	2.7908	3.1286	1.4818	0.0052	0.0879	0.0027
4C-8_87	11.9900	3.6291	1.9709	0.9681	6.2406	5.1130	1.8599	0.4864	0.0670	0.0000	0.0246	0.0000
4B-1_87	8.9152	2.6822	1.4131	0.7078	4.5392	3.6872	1.3366	0.3126	0.0320	0.0000	0.0300	0.0000
3A-10_89	11.7294	3.5645	1.7997	3.2128	5.2199	4.9776	3.7861	3.4166	2.1677	0.1330	0.0774	0.0114
1B-7_87	23.4713	8.2584	0.2254	0.0774	14.9696	13.4217	0.0192	0.0000	0.0000	0.0000	0.0844	0.0738
2B-8_89	8.9882	2.6968	1.6056	2.7523	4.2817	3.8349	3.1881	2.6827	1.5441	0.0668	0.0468	0.0086
3B-17_87	1.4889	0.9608	2.1752	4.7165	9.4260	13.0877	8.3452	12.8487	7.1448	0.2611	0.5293	0.1285
2C-4_89	7.5482	2.2461	1.2313	2.2266	3.4404	3.0659	2.5458	2.1468	1.2730	0.0540	0.0435	0.0018
2B-6_89	8.6107	2.5988	1.4234	2.5710	4.1804	3.7732	2.9864	2.6375	1.6268	0.0804	0.0435	0.0064
3B-6_87	9.5665	2.8220	1.7442	1.8275	4.5792	4.3232	2.2258	2.5601	1.2028	0.0031	0.0848	0.0048
1A-5_89	22.5433	7.6066	0.1541	0.0524	13.8688	12.7476	0.0129	0.0000	0.0114	0.0000	0.0924	0.0649
4B-16_87	2.3127	1.5446	3.0669	3.6336	18.2554	23.3911	10.5452	4.8162	2.4412	0.1990	0.4092	0.2289
2B-17_87	2.2432	1.4574	2.7588	6.1874	15.2354	21.2169	11.1994	19.3341	11.9969	0.5428	0.2899	0.1011
4B-9_87	12.1044	3.6746	1.9982	0.9808	6.3657	5.2182	1.9119	0.4966	0.0811	0.0000	0.0309	0.0000
2B-15_89	12.2334	4.5706	3.8479	8.0521	12.2691	12.1849	10.1624	9.4475	5.6977	0.4578	0.1237	0.0346
4A-2_87	9.3830	2.8236	1.5240	0.7604	4.7902	3.8866	1.4341	0.3383	0.0414	0.0000	0.0320	0.0000
1A-14_87	29.7609	11.6646	0.3959	0.1780	26.6430	25.4293	0.0437	0.0000	0.0132	0.0000	0.1674	0.1769
2B-13_87	15.5537	5.0801	3.3016	3.9225	11.2146	11.2465	5.1532	6.3715	3.3091	0.0331	0.0845	0.0079
3B-11_87	12.7802	3.8332	2.4813	2.5968	6.4698	6.1331	3.1829	3.5291	1.6974	0.0054	0.1098	0.0061

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1C-10_89	30.4409	10.4220	0.2062	0.0844	19.7846	18.2488	0.0195	0.0000	0.0155	0.0000	0.1258	0.0971
2B-7_87	11.7025	3.6030	1.7294	2.4204	7.2316	7.2382	3.2798	4.4467	1.9083	0.0000	0.0246	0.0000
2B-4_87	10.1601	3.0540	1.7713	1.9885	5.5526	5.3748	2.6085	3.1341	1.5412	0.0000	0.0479	0.0000
1C-7_87	25.1576	8.9251	0.1887	0.0524	16.6504	15.2558	0.0210	0.0000	0.0000	0.0000	0.0683	0.0449
1C-4_89	21.8422	7.3838	0.1184	0.0373	13.6786	12.7018	0.0067	0.0000	0.0000	0.0000	0.0619	0.0412
3A-10_87	11.5284	3.4291	2.1560	2.2530	5.6759	5.3721	2.7523	3.0498	1.4470	0.0058	0.0879	0.0027
4A-14_87	18.1237	5.9874	3.8385	2.0868	12.7762	10.9721	4.0932	1.2686	0.3370	0.0000	0.0735	0.0180
2C-10_89	9.5319	2.8745	1.6871	2.9400	4.6483	4.1637	3.4132	2.9101	1.7372	0.1189	0.0458	0.0125
1A-3_87	16.9562	5.8101	0.1738	0.0633	9.8096	8.6602	0.0149	0.0000	0.0061	0.0000	0.0697	0.0453
3C-19_87	0.0314	0.0341	0.2024	1.3102	2.0470	5.1096	5.2866	17.6988	14.4871	0.5486	1.1895	0.3384
3B-18_89	0.1922	0.1969	1.2404	6.2105	5.7461	10.2124	14.1116	22.7376	17.2151	1.2763	0.6964	0.2921
4C-15_87	18.8239	6.4520	4.3982	2.4312	15.0155	13.1520	4.9530	1.5515	0.5150	0.0045	0.1066	0.0368
1B-7_89	26.3667	8.9393	0.1543	0.0602	16.5983	15.3426	0.0228	0.0000	0.0000	0.0000	0.1097	0.0737
3A-18_87	0.8773	0.6593	1.8265	4.4179	8.5342	12.5038	8.2990	13.7118	7.8986	0.2828	0.5712	0.1510
4A-1_87	8.9433	2.6802	1.4410	0.7262	4.5400	3.6687	1.3653	0.3171	0.0382	0.0000	0.0270	0.0000
1B-11_89	33.0666	11.3801	0.2433	0.1000	21.7129	19.9489	0.0244	0.0000	0.0060	0.0000	0.1422	0.1143
1B-2_89	19.0955	6.3935	0.1241	0.0310	11.4536	10.3423	0.0129	0.0000	0.0000	0.0000	0.0654	0.0469
3A-17_87	7.1895	3.1015	3.5667	5.2183	11.8709	13.3804	7.4138	9.4136	4.8727	0.1830	0.3388	0.0760
2C-6_87	10.5554	3.1518	1.7617	2.0961	5.8668	5.7128	2.8362	3.5097	1.5685	0.0000	0.0222	0.0000

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
3C-1_89	7.7205	2.2953	1.1292	1.9689	3.1216	2.9299	2.3073	2.0259	1.1453	0.0361	0.0459	0.0060
4C-1_87	8.5282	2.5665	1.3675	0.6844	4.3278	3.4998	1.2741	0.2899	0.0207	0.0000	0.0289	0.0000
1C-11_89	32.8594	11.3610	0.2300	0.1002	21.9843	20.2998	0.0255	0.0000	0.0000	0.0000	0.1370	0.1051
1B-11_87	28.9803	10.2496	0.3345	0.1242	18.9256	17.1545	0.0331	0.0000	0.0082	0.0000	0.1092	0.0971
2A-7_87	11.0731	3.3307	2.0226	2.1829	6.0289	5.7938	2.7569	3.2341	1.5906	0.0085	0.0581	0.0020
2B-6_87	11.1896	3.3980	1.7359	2.2464	6.4196	6.3165	2.9348	3.7854	1.7328	0.0000	0.0259	0.0000
1A-9_87	29.7070	10.7323	0.2302	0.0693	21.1685	19.8057	0.0247	0.0000	0.0000	0.0000	0.0626	0.0546
1C-13_89	33.7475	11.8029	0.3450	0.1418	24.3240	22.6184	0.0354	0.0000	0.0000	0.0000	0.2064	0.1599
2A-10_87	13.0146	3.9827	2.2535	2.6700	7.5629	7.3641	3.4017	4.2776	2.1396	0.0048	0.0440	0.0000
1C-18_87	2.2691	2.1163	0.1182	0.2116	31.3672	47.1006	0.0924	0.0187	0.0000	0.0000	0.7741	0.7386
1A-16_87	21.8436	10.4956	0.3464	0.2219	36.9971	39.4062	0.0656	0.0000	0.0000	0.0000	0.2704	0.2504
2C-6_89	8.0071	2.4153	1.3337	2.4640	3.9305	3.5665	2.9489	2.6603	1.7183	0.0680	0.0426	0.0054
1C-13_87	32.7320	12.3620	0.3873	0.1708	26.7893	25.2397	0.0383	0.0000	0.0000	0.0000	0.1583	0.1671
1A-12_89	33.2972	11.5117	0.2482	0.1024	22.1062	20.2898	0.0235	0.0000	0.0130	0.0000	0.1440	0.1197
3A-11_87	12.3810	3.7087	2.3777	2.4990	6.2459	5.9182	3.0984	3.4030	1.6267	0.0051	0.1012	0.0060
4B-13_87	17.2367	5.4744	3.2591	1.7223	10.5531	8.9039	3.2871	1.0060	0.2440	0.0000	0.0635	0.0060
1A-6_87	23.0045	8.1413	0.1871	0.0561	15.2610	14.0815	0.0188	0.0000	0.0000	0.0000	0.0465	0.0335
3B-10_89	11.2313	3.4135	1.7611	3.1024	4.9635	4.7234	3.6285	3.2549	2.0262	0.0935	0.0765	0.0114
2B-4_87	10.2445	3.0795	1.5219	2.0169	5.7286	5.6237	2.5274	3.2606	1.3667	0.0000	0.0212	0.0000

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2C-13_87	15.1720	4.8452	3.1215	3.5826	10.1055	9.9687	4.6230	5.6494	2.9186	0.0237	0.0802	0.0086
2A-12_87	15.2901	4.7659	2.7152	3.1496	9.6491	9.6368	4.1810	5.4022	2.9126	0.0000	0.0702	0.0035
3A-13_87	14.4325	4.5194	3.0946	3.4588	8.3692	8.0904	4.1903	4.7366	2.3310	0.0140	0.1434	0.0141
2B-17_89	1.1461	0.8011	2.4676	8.3307	9.3066	12.5705	14.2008	16.8006	10.5398	0.7308	0.3138	0.1545
1A-17_89	21.3116	10.1796	0.2935	0.1897	38.4362	41.9252	0.0486	0.0000	0.0000	0.0000	0.3618	0.3124
2B-19_87	0.0000	0.0000	0.1323	1.2891	1.8669	5.8595	6.7754	27.8040	25.2974	1.0372	0.7082	0.3185
2C-10_89	9.9322	3.0087	1.7257	3.0869	4.9622	4.5143	3.6330	3.1669	1.9758	0.1912	0.0487	0.0115
1B-11_87	29.0673	10.3245	0.3409	0.1355	19.0532	17.2441	0.0292	0.0000	0.0000	0.0000	0.1108	0.0953
2A-4_89	8.1580	2.4496	1.3673	2.4717	4.0150	3.6468	2.9139	2.6402	1.6505	0.0574	0.0258	0.0037
2B-10_89	9.5376	2.8945	1.6973	3.0483	4.7253	4.2598	3.5256	3.0235	1.7913	0.1404	0.0526	0.0099
1A-9_89	27.2791	9.2288	0.2095	0.0817	16.8604	15.2404	0.0189	0.0000	0.0000	0.0000	0.1234	0.0902
2C-11_87	13.0566	3.9923	2.4741	2.6812	7.3772	7.0685	3.3686	3.9588	1.9964	0.0104	0.0717	0.0077
1A-14_87	28.6739	11.2048	0.4108	0.1763	25.3134	24.0003	0.0440	0.0000	0.0000	0.0000	0.1787	0.1584
4C-6_87	10.8654	3.2778	1.7818	0.8830	5.6128	4.5433	1.6855	0.4184	0.0627	0.0000	0.0298	0.0000
2A-12_89	11.8719	3.6620	2.1783	3.9337	6.2772	5.6977	4.5918	4.0128	2.5293	0.2242	0.0600	0.0194
4C-5_87	10.4016	3.1361	1.6779	0.8381	5.3593	4.3448	1.5891	0.3901	0.0618	0.0000	0.0280	0.0000
3C-6_87	10.0157	2.9506	1.8477	1.9077	4.7622	4.4775	2.3271	2.5992	1.2471	0.0046	0.0812	0.0041
2C-1_87	7.6941	2.2949	1.1451	1.4681	4.0731	3.9341	1.8929	2.3369	0.9270	0.0000	0.0072	0.0000
3A-19_89	0.0930	0.1238	1.0555	5.8426	5.2086	9.8907	14.3218	25.1714	20.5633	1.5932	0.7473	0.3255

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1A-19_89	4.5349	3.4796	0.1203	0.2005	35.1809	48.2955	0.0641	0.0125	0.0000	0.0000	0.7120	0.6412
2C-15_87	14.3247	5.1665	3.9072	5.2572	14.5214	15.4873	7.3599	10.0148	5.6917	0.0786	0.1224	0.0182
3C-16_87	8.4973	3.5085	3.6504	5.1602	11.9814	13.2309	7.2710	9.0093	4.6308	0.1842	0.3261	0.0630
1C-11_87	30.8508	11.1364	0.2981	0.1147	21.3907	19.6356	0.0293	0.0000	0.0156	0.0000	0.1108	0.0800
3A-9_89	10.8755	3.2910	1.6501	2.9510	4.7683	4.5384	3.4675	3.1446	2.0193	0.1519	0.0690	0.0092
2C-15_87	14.3100	5.1662	4.0272	5.0789	14.2344	14.8905	6.8878	8.9258	4.8911	0.1378	0.1279	0.0357
2A-7_89	8.5365	2.5648	1.4399	2.6414	4.1738	3.7839	3.0835	2.7540	1.7789	0.0873	0.0340	0.0053
4A-3_87	9.7117	2.9267	1.5944	0.8032	4.9530	4.0125	1.4773	0.3076	0.0281	0.0000	0.0335	0.0000
3B-9_89	10.9952	3.3141	1.6155	2.9221	4.7022	4.4324	3.4418	3.0520	1.9089	0.1412	0.0693	0.0100
1C-8_89	26.3798	8.8680	0.2018	0.0829	16.1183	14.5100	0.0169	0.0000	0.0139	0.0000	0.1206	0.0932
2A-18_87	0.5217	0.4844	1.6866	5.0930	11.5294	19.1223	11.5137	23.8964	16.0170	0.7312	0.3707	0.1426
2A-18_87	0.4931	0.4734	1.6399	4.9379	10.6119	17.3453	10.8314	21.9180	14.2220	0.5998	0.3682	0.1419
1C-11_87	31.0085	11.1926	0.2979	0.1398	21.6090	19.7461	0.0306	0.0000	0.0000	0.0000	0.1149	0.0969
4A-16_87	14.4801	5.8713	5.0749	3.2426	19.0104	18.5101	7.0376	2.3360	1.0190	0.0265	0.1597	0.0697
1A-11_87	31.5138	11.4299	0.2885	0.1067	22.5008	20.8118	0.0310	0.0000	0.0000	0.0000	0.1074	0.0943
2B-12_87	16.2495	5.1107	2.9205	3.4558	10.6981	10.7486	4.6722	5.9699	3.2210	0.0000	0.0583	0.0000
3A-3_89	8.4051	2.5065	1.2417	2.2011	3.4363	3.2291	2.5481	2.2237	1.3109	0.0532	0.0489	0.0038
2A-14_89	15.4123	5.3096	3.6918	7.3672	11.8910	11.4354	9.0564	8.3582	5.3727	0.4966	0.0796	0.0186
1C-1_89	16.6299	5.5472	0.1204	0.0458	9.7673	8.7793	0.0120	0.0000	0.0041	0.0000	0.0779	0.0435

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1C-2_87	14.3883	4.9506	0.1390	0.0509	8.3488	7.3413	0.0114	0.0000	0.0000	0.0000	0.0555	0.0374
2A-9_89	8.8761	2.6628	1.5262	2.7216	4.2593	3.8154	3.1462	2.7165	1.6797	0.0963	0.0397	0.0038
3A-16_87	11.0773	4.2103	3.9474	5.1212	12.0827	13.0931	6.7701	8.2436	4.1815	0.1422	0.2883	0.0611
1A-17_87	12.7619	7.1091	0.3209	0.2307	33.7265	38.4837	0.0680	0.0000	0.0000	0.0000	0.3608	0.3230
1C-2_87	14.1838	4.9174	0.1466	0.0534	8.3018	7.2884	0.0152	0.0000	0.0041	0.0000	0.0531	0.0362
2C-17_87	4.9772	2.6299	3.4832	6.4234	17.1158	21.5540	10.7164	16.6228	9.7572	0.4380	0.2295	0.0747
2B-14_89	14.3205	4.9049	3.6470	7.1258	10.7616	10.1895	8.6460	7.7636	4.6450	0.3762	0.1054	0.0304
3C-1_87	7.1982	2.1010	1.3238	1.3605	3.3211	3.1081	1.6515	1.8240	0.7597	0.0000	0.0584	0.0000
3B-16_89	9.7773	4.1756	4.0738	9.2736	13.4884	14.9739	12.7791	13.1791	8.6908	0.7163	0.2956	0.1189
3C-5_87	9.5860	2.8189	1.7551	1.7963	4.5252	4.2651	2.2484	2.4587	1.1512	0.0000	0.0773	0.0047
3B-6_89	9.2171	2.7598	1.3510	2.3982	3.8221	3.6092	2.7808	2.4492	1.4466	0.0731	0.0516	0.0084
4A-2_87	9.3702	2.8242	1.5145	0.7524	4.7897	3.8867	1.4393	0.3431	0.0414	0.0000	0.0275	0.0000
3A-13_89	15.7756	5.0343	2.8085	5.1733	8.2827	8.0609	6.2168	5.7628	3.6686	0.3468	0.1226	0.0404
3C-3_89	8.2637	2.4471	1.2346	2.1061	3.2670	3.0392	2.3987	2.0196	1.0858	0.0275	0.0501	0.0071
4B-8_87	11.7498	3.5617	1.9272	0.9683	6.1322	5.0245	1.8293	0.4797	0.0622	0.0000	0.0294	0.0022
1A-18_87	3.7659	2.8380	0.1763	0.1945	24.3459	31.7873	0.0672	0.0152	0.0055	0.0000	0.5255	0.5185
1A-10_87	31.8496	11.6135	0.2826	0.1246	23.3595	21.7275	0.0319	0.0000	0.0000	0.0000	0.1035	0.0744
2B-1_89	7.0663	2.1192	1.1450	2.1231	3.4117	3.0970	2.5036	2.2359	1.3734	0.0412	0.0288	0.0019
1C-17_87	9.8944	6.1219	0.2668	0.2389	36.3791	43.3356	0.0740	0.0000	0.0204	0.0000	0.4243	0.4006

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1C-12_89	33.4837	11.5894	0.2592	0.0941	22.4586	20.7227	0.0281	0.0000	0.0000	0.0000	0.1494	0.1110
2C-19_87	0.0448	0.0836	0.7741	3.3703	6.1834	12.7056	9.6447	23.8850	16.5208	0.6410	0.4588	0.1896
2B-5_87	10.5635	3.1831	1.8055	1.9870	5.8491	5.6121	2.5644	3.0635	1.5757	0.0000	0.0373	0.0018
1B-17_87	17.7253	8.9137	0.3711	0.2368	34.2024	37.0464	0.0628	0.0000	0.0072	0.0000	0.3025	0.2711
2A-10_89	9.4449	2.8402	1.7399	2.9904	4.6090	4.1255	3.4623	2.9615	1.8523	0.1119	0.0569	0.0080
1C-3_89	20.2995	6.8206	0.1375	0.0351	12.4208	11.4039	0.0145	0.0000	0.0000	0.0000	0.0804	0.0425
3C-7_89	9.7573	2.9350	1.4642	2.5670	4.1531	3.9176	2.9888	2.6367	1.6742	0.1449	0.0620	0.0111
1B-8_87	27.0757	9.6854	0.2079	0.0694	18.7387	17.4458	0.0222	0.0000	0.0000	0.0000	0.0753	0.0451
1A-3_89	20.9096	7.1349	0.1512	0.0560	13.2797	12.1326	0.0154	0.0000	0.0055	0.0000	0.0984	0.0615
1A-10_87	30.9071	11.2030	0.2486	0.0718	21.9385	20.4088	0.0321	0.0000	0.0000	0.0000	0.0714	0.0763
1B-2_87	14.9669	5.1459	0.1506	0.0516	8.6392	7.5689	0.0138	0.0000	0.0000	0.0000	0.0658	0.0417
2B-14_87	15.7759	5.5173	3.9671	4.9819	14.4369	15.1356	6.8937	9.1390	5.1178	0.0875	0.1158	0.0245
3A-7_87	10.3303	3.0491	1.8961	1.9273	4.9515	4.6683	2.4574	2.6944	1.2977	0.0046	0.0900	0.0046
3A-17_89	5.1314	2.5745	3.5533	9.1606	12.0599	14.5044	13.4891	14.4085	9.1985	0.6900	0.3493	0.1394
3A-10_89	11.5337	3.4937	1.8032	3.1719	5.0654	4.7962	3.7372	3.2953	2.0299	0.1528	0.0765	0.0096
2C-1_89	6.8420	2.0391	1.0898	2.0709	3.2863	2.9676	2.4343	2.2232	1.3231	0.0313	0.0197	0.0000
1B-13_87	32.0571	11.8212	0.4085	0.1715	24.1897	22.4548	0.0403	0.0000	0.0000	0.0000	0.1462	0.1231
3A-1_87	7.2314	2.1176	1.2948	1.3611	3.3352	3.1297	1.6387	1.8108	0.8115	0.0035	0.0567	0.0000
1C-11_87	30.1099	10.7680	0.3183	0.1327	20.3292	18.6543	0.0276	0.0000	0.0134	0.0000	0.1113	0.0902

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
3A-3_87	8.7090	2.5554	1.5570	1.6414	4.0873	3.8348	2.0595	2.2600	0.9994	0.0047	0.0723	0.0000
2C-1_87	7.8688	2.3687	1.1188	1.5031	4.2541	4.1219	1.8700	2.3278	0.9291	0.0000	0.0118	0.0000
2C-3_87	9.9698	2.9958	1.6773	1.9423	5.5056	5.3572	2.5845	3.1614	1.4644	0.0000	0.0316	0.0000
1C-18_89	1.2140	1.3437	0.0575	0.1571	28.8440	50.0075	0.0734	0.0379	0.0000	0.0033	1.0744	0.9912
4A-9_87	12.2935	3.7433	2.0763	1.0392	6.5891	5.4370	2.0080	0.5560	0.0972	0.0000	0.0290	0.0020
4C-3_87	9.8668	2.9637	1.5719	0.7870	5.0307	4.0597	1.4682	0.3497	0.0409	0.0000	0.0366	0.0000
2A-11_87	12.7158	3.8791	2.4220	2.5943	7.1500	6.8328	3.2317	3.7913	1.8536	0.0064	0.0644	0.0060
3C-15_87	13.3753	4.6728	3.8136	4.5863	11.0854	11.3898	5.9295	6.8735	3.4672	0.0635	0.2332	0.0361
2A-8_87	11.3983	3.4555	2.1228	2.2938	6.3111	6.0663	2.9052	3.4493	1.7240	0.0075	0.0587	0.0042
4A-13_87	17.0220	5.4278	3.4011	1.7212	10.6016	8.8765	3.4133	1.0356	0.3058	0.0000	0.0627	0.0170
3B-12_89	12.7874	3.9356	2.0764	3.6945	5.8831	5.6493	4.3994	4.0068	2.6728	0.2497	0.0869	0.0205
1C-7_87	24.6432	8.7228	0.2098	0.0264	16.2176	14.9364	0.0197	0.0000	0.0000	0.0000	0.0542	0.0390
3C-18_87	0.3868	0.3426	1.2483	3.7427	6.8109	11.0530	7.9780	14.8988	9.0658	0.3241	0.6745	0.1817
3C-5_87	9.5935	2.8228	1.7379	1.8219	4.5336	4.2627	2.2422	2.4691	1.1215	0.0000	0.0711	0.0045
2A-3_87	9.7565	2.9378	1.5693	1.8866	5.3325	5.1504	2.4079	2.9487	1.3101	0.0000	0.0307	0.0000
1C-4_89	21.7734	7.3358	0.1481	0.0452	13.4448	12.2510	0.0149	0.0000	0.0115	0.0000	0.0977	0.0567
2B-2_87	9.4558	2.8475	1.5903	1.8253	5.2091	5.0763	2.3856	2.9762	1.4216	0.0000	0.0329	0.0000
2A-7_87	11.8531	3.5996	2.0910	2.3648	6.7718	6.6140	3.0328	3.7093	1.8953	0.0000	0.0498	0.0025
3B-5_87	9.3652	2.7532	1.6738	1.7627	4.4230	4.1536	2.1469	2.3972	1.1223	0.0000	0.0749	0.0024

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
3C-17_87	3.3109	1.7745	2.8240	5.1265	11.0343	13.8339	8.1843	11.5435	6.2216	0.2353	0.4550	0.1165
3C-4_87	9.0004	2.6408	1.6516	1.7007	4.2431	3.9926	2.1166	2.3283	1.0558	0.0000	0.0727	0.0000
3B-14_89	16.7646	5.5764	3.4147	6.4172	10.1508	10.0144	7.8877	7.3111	4.7185	0.4054	0.1663	0.0562
2B-15_87	12.7332	4.9463	4.2232	6.0616	16.4444	18.1842	8.6531	12.1458	7.1136	0.1006	0.1471	0.0374
1B-6_87	22.3495	7.8850	0.1764	0.0553	14.3308	12.9969	0.0214	0.0000	0.0000	0.0000	0.0589	0.0267
3B-14_87	14.7009	4.9378	3.7344	4.2283	10.4320	10.3353	5.3125	6.0198	3.0436	0.0397	0.2080	0.0203
2A-5_87	10.4886	3.2043	1.6063	2.0686	6.1325	6.0518	2.7485	3.5281	1.6949	0.0000	0.0348	0.0000
4A-15_87	18.9344	6.6028	4.6236	2.6149	15.9366	14.1608	5.3049	1.7131	0.5802	0.0053	0.1117	0.0403
2A-18_87	0.4775	0.4602	1.5945	5.0105	11.0161	18.3671	11.4411	23.8021	16.4349	0.7924	0.3689	0.1405
1B-16_89	18.5968	9.4969	0.2027	0.1414	42.3557	48.1772	0.0570	0.0000	0.0000	0.0000	0.3891	0.3475
2C-11_89	10.0420	3.0832	1.7455	3.1427	5.2632	4.8206	3.7318	3.3311	2.1289	0.2037	0.0558	0.0133
4A-9_87	12.2655	3.7400	2.0545	1.0218	6.5827	5.4339	1.9812	0.5602	0.0985	0.0000	0.0337	0.0041
2A-11_89	11.3982	3.5101	2.0146	3.7162	6.0105	5.4975	4.3853	3.9457	2.5743	0.2145	0.0647	0.0179
1C-10_87	29.9602	10.7927	0.2685	0.1050	20.8094	19.1368	0.0275	0.0000	0.0000	0.0000	0.1061	0.0844
4B-13_87	17.2025	5.4578	3.2579	1.7053	10.5472	8.8959	3.3150	1.0120	0.2061	0.0000	0.0591	0.0081
3A-19_89	0.0979	0.1255	1.0680	5.9022	5.3072	10.0774	14.4333	25.3001	20.5068	1.5753	0.7536	0.3337
4C-13_87	16.6508	5.2781	3.1235	1.6404	10.1082	8.4995	3.1180	0.9203	0.2041	0.0033	0.0515	0.0055
4A-12_87	14.5393	4.4947	2.5545	1.2949	8.1608	6.7617	2.5280	0.6952	0.1452	0.0000	0.0365	0.0023
2A-10_89	9.4260	2.8431	1.7002	2.9992	4.5779	4.1202	3.4578	2.9536	1.7972	0.1616	0.0568	0.0081

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2B-8_87	12.5149	3.8383	2.1221	2.5328	7.3377	7.1931	3.3084	4.1269	2.1273	0.0000	0.0426	0.0000
2B-6_89	8.3495	2.4957	1.4024	2.5119	3.9585	3.5271	2.8950	2.4816	1.4869	0.0638	0.0414	0.0041
1B-15_89	31.0459	13.2989	0.2746	0.1753	41.1231	42.9781	0.0453	0.0000	0.0000	0.0000	0.2552	0.2373
1B-5_87	20.0934	7.0366	0.1823	0.0684	12.5877	11.2659	0.0185	0.0000	0.0000	0.0000	0.0805	0.0547
4C-5_87	10.3423	3.1183	1.6707	0.8356	5.3203	4.3187	1.5820	0.3955	0.0495	0.0000	0.0272	0.0020
2C-12_87	14.9659	4.6738	2.7516	3.2148	9.4397	9.3950	4.2761	5.2874	2.7877	0.0136	0.0721	0.0000
2C-16_89	7.3346	3.2073	3.8835	8.9638	12.3048	13.2423	12.1822	12.0198	7.2752	0.5455	0.1881	0.0960
2A-17_87	4.4064	2.3185	3.3153	6.0693	15.1418	19.0207	9.9943	15.4357	9.0817	0.3993	0.2397	0.0765
2A-16_87	9.9563	4.1931	4.0843	5.9979	16.5522	18.7998	8.8503	12.6722	7.2994	0.2219	0.1687	0.0474
2A-3_87	9.7858	2.9576	1.5320	1.8629	5.4843	5.3120	2.4108	3.1061	1.2854	0.0000	0.0230	0.0000
3A-12_89	13.0898	4.0140	2.1261	3.7800	5.9991	5.7028	4.4422	3.9449	2.4524	0.2124	0.0866	0.0194
1A-10_89	28.7019	9.7954	0.1875	0.0765	18.4298	16.9590	0.0206	0.0000	0.0000	0.0000	0.1133	0.0802
3C-12_89	11.9215	3.6550	1.8586	3.3988	5.4789	5.2670	4.0543	3.6658	2.3760	0.2029	0.0798	0.0165
2A-15_89	13.1071	4.8051	3.9651	7.9741	12.1858	11.9020	9.8747	8.8334	5.1515	0.4082	0.1219	0.0382
1B-14_87	30.8505	11.7893	0.4085	0.1733	26.0042	24.6057	0.0444	0.0000	0.0098	0.0000	0.1715	0.1488
3B-6_89	9.2041	2.7522	1.3589	2.4337	3.8503	3.6207	2.8174	2.4807	1.5402	0.0864	0.0606	0.0107
1B-1_87	16.5124	5.9917	0.1636	0.0564	11.9746	11.2380	0.0188	0.0000	0.0000	0.0000	0.0685	0.0528
2B-4_87	10.3348	3.1153	1.7044	2.0586	5.6950	5.5852	2.6877	3.3549	1.6053	0.0000	0.0242	0.0000
4C-15_87	18.8878	6.4760	4.4320	2.4634	15.0650	13.2205	4.9579	1.5775	0.5048	0.0114	0.0970	0.0312

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2C-7_87	10.5906	3.1909	1.9335	2.1047	5.7207	5.5020	2.6718	3.2299	1.5707	0.0000	0.0535	0.0021
1A-8_89	25.8442	8.7223	0.1401	0.0434	16.1018	15.0091	0.0174	0.0000	0.0000	0.0000	0.0856	0.0634
2C-11_89	9.7533	2.9805	1.7118	3.0709	5.0159	4.5395	3.6036	3.1874	1.9974	0.1856	0.0578	0.0152
2C-8_87	10.5634	3.1623	1.9566	2.0593	5.5586	5.2758	2.5466	2.9123	1.4218	0.0060	0.0587	0.0020
1A-19_87	0.3795	0.5529	0.0330	0.1267	19.2812	35.7095	0.0733	0.0258	0.0000	0.0033	1.1392	1.0588
1A-16_87	20.0038	9.5007	0.3855	0.2275	32.1967	33.5244	0.0597	0.0000	0.0000	0.0000	0.2692	0.2319
3C-13_87	14.7194	4.6050	3.1502	3.4679	8.5669	8.3312	4.3078	4.7553	2.3623	0.0200	0.1471	0.0180
3C-8_89	9.9739	3.0101	1.5209	2.6651	4.2825	4.0674	3.1662	2.8034	1.7805	0.1521	0.0643	0.0081
3B-13_87	15.1477	4.7853	3.3078	3.6768	9.0858	8.8593	4.5427	5.0659	2.5105	0.0130	0.1608	0.0174
4A-18_87	0.3427	0.3983	1.6350	2.9059	12.9625	21.9646	10.4555	6.4879	3.5967	0.3182	0.6293	0.3802
2C-14_87	15.3657	5.2637	3.6586	4.6068	13.0292	13.5349	6.2416	8.2385	4.5430	0.0376	0.0866	0.0088
3A-18_87	0.8821	0.6484	1.7951	4.3518	8.3575	12.5726	8.1425	13.7226	7.7963	0.2793	0.5740	0.1566
2B-12_87	14.6049	4.5591	2.8344	3.1737	9.0113	8.8689	4.1531	5.0166	2.6569	0.0129	0.0719	0.0060
1C-17_87	9.5824	5.8896	0.2950	0.2377	33.7691	42.0507	0.0709	0.0160	0.0000	0.0000	0.4188	0.3918
2C-18_89	0.0167	0.0308	0.5965	4.1687	3.0714	6.5474	12.1062	24.0420	20.1516	1.5083	0.5827	0.2890
3B-3_87	8.7095	2.5582	1.6161	1.6611	4.1004	3.8556	2.0914	2.3093	1.0311	0.0000	0.0686	0.0000
2B-16_87	5.8484	2.8158	3.5629	5.8693	15.0086	17.8451	9.1901	13.6384	7.7330	0.3572	0.2271	0.0663
3A-14_89	16.5681	5.5025	3.4063	6.4509	10.0694	9.9532	7.8953	7.4141	4.6958	0.3948	0.1552	0.0539
3A-14_87	13.8606	4.5086	3.2123	3.7092	8.9988	5.3470	4.5802	5.2468	2.5714	0.0236	0.1668	0.0178

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2C-16_87	10.8489	4.3740	4.0538	5.5352	15.3925	16.7987	7.9875	10.8045	5.9077	0.2568	0.1686	0.0463
3B-7_89	10.3913	3.1231	1.5406	2.7304	4.4445	4.2046	3.1984	2.8815	1.8351	0.0989	0.0648	0.0089
3B-2_89	8.0507	2.3851	1.1781	2.0806	3.2470	3.0417	2.4182	2.1320	1.2407	0.0329	0.0503	0.0054
2A-11_87	13.5053	4.1579	2.5446	2.8017	7.9445	7.7066	3.6130	4.3271	2.2247	0.0000	0.0580	0.0074
1A-15_89	33.3996	12.9240	0.2901	0.1490	31.8374	31.2824	0.0378	0.0000	0.0000	0.0000	0.2321	0.1883
3A-17_89	4.9107	2.4598	3.4010	8.5665	11.1022	13.1501	12.3040	12.6327	7.5492	0.5325	0.3532	0.1297
3C-6_87	10.0105	2.9545	1.8453	1.9080	4.7680	4.4854	2.3799	2.6065	1.2312	0.0034	0.0783	0.0025
1C-6_89	23.9527	8.1055	0.1281	0.0349	15.0780	14.0446	0.0179	0.0000	0.0000	0.0000	0.0688	0.0445
3A-11_89	11.8589	3.6441	1.8895	3.3744	5.4615	5.2305	4.0014	3.6095	2.3304	0.1710	0.0739	0.0130
2A-9_89	8.8221	2.6500	1.5429	2.7054	4.2405	3.8049	3.1601	2.7079	1.7046	0.0662	0.0557	0.0059
2A-11_89	11.3493	3.4840	2.0355	3.7185	5.9860	5.4625	4.4008	3.9413	2.5252	0.2034	0.0594	0.0149
4B-9_87	12.1710	3.6956	2.0026	0.9985	6.4033	5.2496	1.9089	0.5027	0.0711	0.0000	0.0258	0.0000
1A-18_89	13.1197	7.4544	0.2369	0.2102	40.2910	47.5315	0.0708	0.0000	0.0000	0.0000	0.4506	0.3989
4A-17_87	8.1221	4.0265	4.7128	3.6546	20.6491	21.4681	8.7116	3.1861	1.4701	0.0511	0.2251	0.1073
2A-3_89	7.8829	2.3966	1.1183	2.3488	4.1093	3.8242	2.8440	2.8609	1.5342	0.0000	0.0164	0.0000
3C-14_89	16.6804	5.4728	3.2177	6.0428	9.6415	9.4807	7.3681	6.8170	4.3198	0.3824	0.1440	0.0472
2B-18_87	0.1147	0.1557	1.0315	3.9463	7.7470	15.0248	10.5510	25.2899	17.8191	0.7384	0.4485	0.1779
1B-13_87	32.8422	12.2153	0.4040	0.1775	25.2664	23.4611	0.0394	0.0000	0.0060	0.0000	0.1498	0.1276
2A-18_89	0.2236	0.2300	1.6167	7.6027	7.0771	11.4763	15.7627	22.3691	15.7358	1.1847	0.4054	0.1988

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
4C-17_87	7.5006	3.8521	4.7789	3.8483	21.2568	22.4380	9.1558	3.3607	1.5116	0.0668	0.2273	0.1200
2B-5_89	7.9132	2.3837	1.3292	2.4301	3.8666	3.4999	2.8417	2.5306	1.5633	0.0746	0.0454	0.0059
2A-9_89	8.7603	2.6338	1.5551	2.6777	4.1686	3.7309	3.0878	2.6378	1.5846	0.0847	0.0490	0.0076
4B-7_87	11.4338	3.4626	1.8827	0.9224	5.9673	4.8855	1.7814	0.4611	0.0658	0.0000	0.0198	0.0000
3B-4_89	8.5946	2.5463	1.2518	2.1847	3.4251	3.1801	2.5035	2.1188	1.2314	0.0352	0.0584	0.0066
2C-6_89	8.0536	2.4315	1.3148	2.4395	3.9356	3.5686	2.8597	2.5574	1.5986	0.0841	0.0443	0.0051
2C-8_89	7.6527	2.2867	1.3197	2.3127	3.6220	3.2449	2.6788	2.3148	1.3724	0.0487	0.0329	0.0051
3C-10_89	11.4842	3.4838	1.7284	3.0959	5.1375	4.9034	3.6597	3.3458	2.1486	0.1557	0.0667	0.0052
3A-1_89	7.2543	2.1495	1.0520	1.8069	2.8758	2.6679	2.0601	1.7541	0.9245	0.0195	0.0546	0.0016
1B-14_87	32.8018	12.7870	0.3759	0.1754	29.0801	27.7923	0.0411	0.0000	0.0000	0.0000	0.1678	0.1481
2B-1_87	7.4696	2.2048	1.2237	1.4299	3.8918	3.7479	1.7570	2.2171	0.8571	0.0000	0.0147	0.0000
3C-4_89	8.2239	2.4440	1.2024	2.1314	3.3505	3.1558	2.4805	2.1678	1.3049	0.0248	0.0561	0.0021
4B-10_87	12.8800	3.9236	2.1600	1.0812	6.8941	5.6736	2.0899	0.5656	0.1051	0.0000	0.0496	0.0022
2B-12_89	11.2426	3.4898	2.0384	3.7482	6.0861	5.5732	4.4518	3.9189	2.4572	0.2284	0.0589	0.0099
1B-10_89	31.0696	10.6572	0.2155	0.0929	20.1954	18.5394	0.0270	0.0000	0.0178	0.0000	0.1260	0.1023
3A-10_89	11.5086	3.5035	1.8045	3.1807	5.0867	4.8386	3.7269	3.3533	2.1318	0.1185	0.0784	0.0152
1C-8_87	26.8737	9.5782	0.2446	0.0862	18.1601	16.5291	0.0249	0.0000	0.0000	0.0000	0.0900	0.0701
3C-19_87	0.0278	0.0337	0.1909	1.3038	2.0373	5.0667	5.3033	17.8432	14.5673	0.5393	1.1902	0.3435
1C-6_87	22.3907	7.8960	0.1991	0.0663	14.3222	12.9163	0.0220	0.0000	0.0000	0.0000	0.0714	0.0404

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2A-8_89	8.3247	2.4932	1.4599	2.5020	3.9332	3.5215	2.8726	2.4279	1.3540	0.0165	0.0382	0.0035
3C-12_89	11.9458	3.6645	1.8750	3.3979	5.4645	5.2433	4.0001	3.6389	2.3246	0.1560	0.0804	0.0171
3C-6_89	8.9551	2.6879	1.3630	2.3560	3.7588	3.5516	2.7563	2.4138	1.4730	0.0466	0.0592	0.0087
3A-17_89	5.1186	2.5715	3.5592	9.1761	11.9753	14.3575	13.4333	14.2766	8.9770	0.6564	0.3586	0.1369
1B-1_89	17.0660	5.7126	0.1145	0.0303	10.1824	9.2193	0.0131	0.0000	0.0000	0.0000	0.0746	0.0382
3A-19_89	0.0961	0.1192	1.0143	5.5289	4.8059	9.0130	13.3092	22.6415	17.4247	1.2791	0.7414	0.3292
1B-2_87	15.0214	5.1664	0.1494	0.0572	8.6676	7.6051	0.0123	0.0000	0.0056	0.0000	0.0683	0.0447
2C-12_87	14.8637	4.6539	2.8266	3.2767	9.5121	9.5265	4.4720	5.7440	3.1326	0.0067	0.0645	0.0000
3B-5_89	8.2455	2.4488	1.2213	2.0840	3.3251	3.0960	2.4037	2.0498	1.1764	0.0276	0.0597	0.0066
3C-18_89	2.4181	1.4652	2.8507	8.6992	10.6772	14.0924	14.0921	16.3415	10.4592	0.7431	0.4420	0.1806
3B-2_87	8.1966	2.4061	1.4712	1.5485	3.8391	3.5637	1.8714	2.1235	0.9414	0.0000	0.0639	0.0000
3B-11_89	12.6970	3.8953	1.9845	3.4792	5.7355	5.4812	4.1112	3.6759	2.3812	0.1997	0.0771	0.0172
3A-9_89	10.9601	3.3148	1.6088	2.9888	4.8478	4.6275	3.5187	3.2231	2.0607	0.0789	0.0583	0.0098
1B-6_89	23.8547	8.0085	0.1741	0.0770	14.2968	12.9192	0.0165	0.0000	0.0000	0.0000	0.0994	0.0711
3A-11_89	11.7628	3.5979	1.8547	3.3660	5.3719	5.1555	3.9856	3.6018	2.2456	0.1702	0.0777	0.0131
4C-18_87	1.5540	1.2232	2.9265	3.6619	17.7280	23.5457	10.8176	5.1390	2.5219	0.2056	0.4154	0.2363
3C-4_89	8.1964	2.4460	1.2344	2.1639	3.3637	3.1566	2.5212	2.2192	1.3332	0.0265	0.0507	0.0074
1A-7_87	24.6134	8.7119	0.2087	0.0734	15.9545	14.4389	0.0193	0.0000	0.0000	0.0000	0.0778	0.0642
4A-14_87	13.0900	6.0343	3.8303	2.0771	12.8619	11.0374	4.1187	1.2899	0.3311	0.0000	0.0843	0.0180

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
3C-16_89	13.1570	5.0036	4.0321	8.3155	12.3547	12.8638	10.6978	10.2478	6.2995	0.5009	0.2310	0.0865
4A-10_87	13.3711	4.0840	2.2506	1.1342	7.1907	5.9266	2.1745	0.6142	0.1318	0.0000	0.0414	0.0052
1C-2_87	14.3665	4.9388	0.1468	0.0509	8.3335	7.3310	0.0113	0.0000	0.0032	0.0000	0.0588	0.0361
1C-9_89	28.3100	9.5835	0.1834	0.0574	17.8614	16.5251	0.0216	0.0000	0.0000	0.0000	0.1125	0.0869
2B-17_87	2.2442	1.4520	2.7873	6.0194	14.8806	20.5087	11.0485	18.5618	11.2397	0.4918	0.2812	0.1090
1B-2_87	15.0600	5.1731	0.1550	0.0560	8.6754	7.6193	0.0154	0.0000	0.0073	0.0000	0.0746	0.0411
1A-15_87	26.4090	11.1068	0.3960	0.1931	29.3863	28.9908	0.0504	0.0000	0.0059	0.0000	0.2144	0.1862
1A-6_89	23.3954	7.8602	0.1698	0.0644	14.1241	12.7343	0.0176	0.0000	0.0091	0.0000	0.0965	0.0731
4C-16_87	16.0150	6.2208	5.1920	3.1220	18.8519	18.1012	6.8484	2.2410	0.9090	0.0163	0.1512	0.0653
3C-11_87	11.9896	3.5897	2.2845	2.4460	6.0323	5.7503	2.9831	3.2739	1.5034	0.0091	0.0930	0.0030
4C-1_87	8.6369	2.5878	1.3740	0.6845	4.3581	3.5240	1.2874	0.3050	0.0243	0.0000	0.0241	0.0000
1C-16_89	22.4160	10.6486	0.2786	0.1783	40.0960	43.7230	0.0428	0.0000	0.0129	0.0000	0.3481	0.3060
1A-7_87	25.5840	9.0904	0.2214	0.0736	16.8418	15.3165	0.0202	0.0000	0.0000	0.0000	0.0832	0.0673
2A-12_87	13.5245	4.1526	2.6130	2.7356	7.7348	7.3439	3.4160	4.0102	1.9432	0.0201	0.0762	0.0164
2B-7_89	8.8118	2.6521	1.4988	2.6401	4.2293	3.8123	3.0756	2.6436	1.6122	0.1086	0.0373	0.0052
4B-4_87	10.2282	3.0838	1.6638	0.8284	5.2271	4.2291	1.5503	0.3792	0.0458	0.0000	0.0326	0.0000
3B-8_89	10.4669	3.1479	1.5434	2.7670	4.4583	4.2231	3.2102	2.8734	1.8222	0.1216	0.0623	0.0107
2A-15_89	12.8384	4.6964	3.9182	7.9447	11.8881	11.6145	9.8066	8.8128	5.1526	0.4038	0.1196	0.0366
1B-4_89	21.7804	7.3172	0.1374	0.0390	13.3185	12.2308	0.0143	0.0000	0.0077	0.0000	0.0880	0.0541

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2A-2_89	7.4231	2.2348	1.1000	2.1612	3.6482	3.3378	2.5977	2.3643	1.1864	0.0091	0.0107	0.0000
1C-12_89	34.9634	12.1577	0.2409	0.0849	24.1507	22.6443	0.0229	0.0000	0.0000	0.0000	0.1425	0.1092
2A-14_89	15.2587	5.2362	3.7253	7.2279	11.6237	11.1206	8.7864	7.9626	4.9213	0.4160	0.0936	0.0315
1A-16_89	28.4590	12.0405	0.3122	0.1902	35.7734	36.5939	0.0498	0.0000	0.0000	0.0000	0.2888	0.2467
2B-18_87	0.1096	0.1479	0.9780	3.7853	7.1854	13.7444	10.0138	23.4386	16.0012	0.6519	0.4459	0.1742
1B-2_89	18.5625	6.1866	0.1371	0.0424	10.9104	9.7843	0.0122	0.0000	0.0000	0.0000	0.0731	0.0504
4B-15_87	6.6654	3.5211	4.3667	3.6841	20.7297	22.3869	9.1342	3.5372	1.6985	0.0701	0.2635	0.1404
3C-16_89	13.0310	4.9430	3.9662	8.1077	12.0969	12.7250	10.4261	9.7570	5.8205	0.4379	0.2360	0.0757
3C-15_89	16.5925	5.6616	3.6345	7.0623	10.9686	10.9260	8.7433	8.1726	5.1778	0.4259	0.1733	0.0482
4C-4_87	10.1552	3.0614	1.6561	0.8165	5.1937	4.2074	1.5585	0.3814	0.0511	0.0000	0.0307	0.0000
3A-1_89	7.2763	2.1560	1.0476	1.8310	2.8956	2.6914	2.1143	1.7836	0.9376	0.0255	0.0428	0.0031
1A-4_89	21.4971	7.2336	0.1382	0.0424	13.1635	12.0602	0.0129	0.0000	0.0000	0.0000	0.0744	0.0490
2A-19_87	0.0000	0.0332	0.4750	2.6788	4.9237	11.7369	9.3653	28.5247	22.6188	0.9634	0.5584	0.2455
1B-3_89	19.6275	6.5613	0.1378	0.0473	11.6126	10.4111	0.0140	0.0000	0.0105	0.0000	0.0766	0.0530
1A-6_89	23.8754	8.0403	0.1666	0.0612	14.5404	13.1632	0.0150	0.0000	0.0060	0.0000	0.1038	0.0711
1B-4_89	20.3936	6.8223	0.1410	0.0512	12.1461	10.9332	0.0115	0.0000	0.0081	0.0000	0.0870	0.0553
2B-16_87	5.7917	2.8376	3.5301	5.9607	15.2226	18.3812	9.5538	14.2827	8.3418	0.3518	0.2180	0.0716
4C-3_87	9.9048	2.9745	1.5802	0.7929	5.0365	4.0860	1.4828	0.3378	0.0388	0.0000	0.0174	0.0000
3B-13_89	15.4787	4.9383	2.7523	5.0012	8.0791	7.8101	5.9982	5.5257	3.6306	0.3351	0.1274	0.0377

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1A-1_89	17.6016	5.8951	0.1141	0.0295	10.5620	9.6581	0.0126	0.0000	0.0000	0.0000	0.0781	0.0406
3A-17_87	7.1577	3.0942	3.5886	5.2408	11.8085	13.3138	7.3790	9.4165	4.8887	0.1812	0.3421	0.0710
1A-11_89	32.9847	11.3862	0.2218	0.0924	22.2237	20.6675	0.0200	0.0000	0.0000	0.0000	0.1373	0.1021
1A-2_89	18.2404	6.0623	0.1241	0.0384	10.6126	9.5134	0.0120	0.0000	0.0000	0.0000	0.0668	0.0374
3A-11_87	12.3146	3.6837	2.3658	2.5148	6.1913	5.8810	3.0767	3.4145	1.6360	0.0047	0.0970	0.0056
1B-17_89	9.4612	6.0364	0.1840	0.1951	40.6990	50.5135	0.0646	0.0000	0.0000	0.0000	0.5151	0.4608
1B-12_89	32.6996	11.3297	0.2566	0.1090	21.9535	20.1191	0.0215	0.0000	0.0187	0.0000	0.1559	0.1329
2B-14_89	14.6483	5.0235	3.6965	7.1703	11.1161	10.6530	8.8329	8.0554	4.9958	0.4287	0.0820	0.0222
3A-4_89	8.0694	2.3898	1.1972	2.0491	3.2073	2.9761	2.3435	1.9530	1.0471	0.0109	0.0495	0.0054
2B-3_89	7.3784	2.1947	1.2454	2.2322	3.4583	3.1053	2.5767	2.2546	1.3802	0.0455	0.0314	0.0039
2B-17_87	2.1217	1.3672	2.6797	5.8483	13.6917	18.7055	10.3744	17.7527	10.5635	0.4566	0.2845	0.1100
4A-15_87	18.8381	6.5748	4.6326	2.6127	15.8657	14.1083	5.2916	1.7052	0.5878	0.0053	0.1083	0.0421
3B-17_89	2.5234	1.5241	3.0155	8.9970	11.0428	14.5370	14.5565	17.0862	11.1507	0.8184	0.4620	0.1793
4A-16_87	14.4220	5.8566	5.0242	3.2265	18.9162	18.3798	6.9609	2.3129	1.0004	0.0255	0.1646	0.0740
1B-15_89	28.9463	12.2327	0.2884	0.1342	36.7026	37.8908	0.0461	0.0000	0.0000	0.0000	0.2554	0.2297
4B-4_87	10.2470	3.0881	1.6684	0.8482	5.2447	4.2436	1.5448	0.3962	0.0437	0.0000	0.0322	0.0000
2A-9_87	12.1595	3.6981	2.2230	2.4153	6.7178	6.4597	3.0482	3.5628	1.8094	0.0082	0.0707	0.0044
1C-15_87	27.3416	11.6814	0.4112	0.2034	31.3629	30.9573	0.0556	0.0000	0.0072	0.0000	0.2195	0.1964
1A-17_87	12.6440	7.0522	0.3045	0.2297	33.0538	37.9422	0.0671	0.0000	0.0000	0.0000	0.3570	0.3274

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2C-16_89	7.4716	3.2902	4.0020	9.3137	12.8190	13.7565	12.8042	12.7427	7.9620	0.6275	0.1949	0.0870
3C-1_87	7.2269	2.1128	1.2743	1.3227	3.3469	3.0942	1.6631	1.8254	0.7554	0.0000	0.0566	0.0000
4A-2_87	9.3111	2.7983	1.5474	0.7618	4.7522	3.8479	1.4579	0.3378	0.0380	0.0000	0.0298	0.0000
4C-14_87	18.4825	6.0552	3.8310	2.0715	12.7861	11.0140	4.0429	1.2735	0.3524	0.0034	0.0787	0.0186
1B-14_89	34.1627	12.9439	0.2935	0.1276	30.7472	29.8609	0.0379	0.0000	0.0393	0.0000	0.1971	0.1822
1C-10_89	30.8294	10.5766	0.1863	0.0749	20.1075	18.6184	0.0221	0.0000	0.0000	0.0000	0.1182	0.0977
1A-5_89	22.3903	7.5640	0.1488	0.0519	13.7990	12.7055	0.0131	0.0000	0.0000	0.0000	0.0820	0.0583
1C-12_87	31.0802	11.1603	0.3555	0.1382	21.2421	19.4217	0.0332	0.0000	0.0083	0.0000	0.1202	0.1111
2A-18_89	0.2235	0.2332	1.6091	7.5557	7.0439	11.4834	15.6389	22.1203	15.4244	1.1333	0.3951	0.1971
1A-6_87	23.0665	8.2140	0.1967	0.0486	15.4141	14.1944	0.0077	0.0000	0.0000	0.0000	0.0504	0.0401
3A-15_87	13.6577	4.6998	3.6493	4.4222	10.6329	10.7294	5.6526	6.4702	3.2772	0.0428	0.2166	0.0352
3B-12_87	12.6798	3.8287	2.5193	2.6346	6.5213	6.1850	3.2335	3.5588	1.7158	0.0096	0.1075	0.0029
1A-19_87	0.3673	0.5587	0.0234	0.1361	20.4873	38.6535	0.0659	0.0066	0.0000	0.0000	1.1624	1.1411
3A-18_87	0.8835	0.6614	1.8660	4.4382	8.6356	12.6759	8.2964	13.6937	7.9237	0.2873	0.5775	0.1392
3B-17_87	1.4724	0.9430	2.1680	4.7101	9.2938	12.8860	8.3197	12.7932	7.1179	0.2619	0.5255	0.1361
1A-1_87	13.5504	4.6641	0.1375	0.0533	7.8187	6.8764	0.0116	0.0000	0.0080	0.0000	0.0562	0.0337
3C-2_87	8.2486	2.4224	1.4833	1.5660	3.8994	3.6376	1.9874	2.2050	1.0087	0.0000	0.0687	0.0000
2A-4_87	10.0151	3.0233	1.6144	1.9467	5.5726	5.4606	2.5552	3.2083	1.4619	0.0000	0.0293	0.0000
1C-4_87	19.1738	6.7084	0.1841	0.0643	11.9704	10.6284	0.0178	0.0000	0.0000	0.0000	0.0741	0.0444

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
3C-13_89	15.3983	4.8658	2.7310	4.8786	7.8868	7.6351	5.8428	5.3090	3.2912	0.2981	0.1200	0.0335
4B-1_87	8.8419	2.6587	1.4165	0.7079	4.4996	3.6531	1.3418	0.3086	0.0322	0.0000	0.0325	0.0000
3A-13_87	14.2889	4.5024	3.0888	3.4132	8.3266	8.0398	4.2212	4.7327	2.3429	0.0153	0.1519	0.0120
1B-11_89	34.2015	11.9862	0.1838	0.0528	24.3915	23.4137	0.0130	0.0000	0.0000	0.0000	0.1221	0.0909
1C-14_89	33.5334	12.7585	0.2721	0.1383	30.2118	29.2829	0.0312	0.0000	0.0062	0.0000	0.2002	0.1639
1C-5_89	22.5748	7.6111	0.1475	0.0534	13.9459	12.7714	0.0153	0.0000	0.0072	0.0000	0.0941	0.0674
4A-18_87	0.3422	0.3951	1.6271	2.9053	12.8572	21.8931	10.4672	6.4720	3.5689	0.3096	0.6466	0.3699
1B-10_89	31.5951	10.8446	0.2109	0.0618	20.7568	19.2795	0.0275	0.0000	0.0000	0.0000	0.1046	0.0849
3C-12_87	11.4916	3.4730	2.2512	2.4009	5.9376	5.6715	2.9464	3.2951	1.5533	0.0053	0.0901	0.0027
1B-3_89	19.8304	6.6417	0.1330	0.0475	11.8433	10.6796	0.0142	0.0000	0.0000	0.0000	0.0804	0.0546
2A-15_89	13.2581	4.8691	3.9547	8.1385	12.4638	12.2296	10.1037	9.1791	5.5019	0.4488	0.1233	0.0441
3C-18_89	2.4417	1.4802	2.9013	8.8174	10.9032	14.4375	14.4062	16.9054	11.0447	0.8094	0.4485	0.1821
2B-14_87	14.8870	5.1247	3.7928	4.5698	12.6823	12.9306	6.0770	7.7430	4.0867	0.0673	0.1081	0.0202
4A-7_87	11.3394	3.4366	1.8733	0.9234	5.8888	4.8295	1.7782	0.4469	0.0595	0.0000	0.0355	0.0021
3C-4_89	8.1781	2.4371	1.2024	2.1176	3.3193	3.0986	2.4519	2.0964	1.1813	0.0176	0.0561	0.0057
4A-3_87	9.8085	2.9453	1.6045	0.7835	4.9947	4.0872	1.4447	0.3138	0.0242	0.0000	0.0371	0.0000
2C-9_89	8.2928	2.5065	1.4510	2.5676	3.9877	3.5846	2.9984	2.6066	1.5630	0.0322	0.0476	0.0038
1C-14_87	31.3857	12.4210	0.4189	0.1988	29.3773	28.1840	0.0444	0.0000	0.0000	0.0000	0.1829	0.1651
3B-7_87	10.7115	3.1713	1.9501	2.0011	5.1351	4.7913	2.4317	2.6001	1.2502	0.0040	0.0784	0.0023

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2B-11_89	10.6673	3.2795	1.9594	3.5567	5.6426	5.1639	4.2086	3.7310	2.4025	0.1846	0.0510	0.0141
1A-11_87	31.1725	11.2831	0.2989	0.0957	22.1964	20.6099	0.0321	0.0000	0.0000	0.0000	0.0965	0.0825
3C-9_89	10.4418	3.1569	1.5845	2.8076	4.5128	4.2802	3.2843	2.9310	1.8830	0.1317	0.0591	0.0089
2A-17_89	2.4265	1.4325	3.0713	9.1087	11.0337	13.6071	14.0533	15.2918	9.4089	0.6761	0.2648	0.1334
3C-14_89	16.5554	5.4223	3.1916	5.9783	9.5435	9.3732	7.2782	6.7032	4.2635	0.3725	0.1500	0.0451
2A-10_87	12.7943	3.8969	2.3563	2.5373	7.2210	6.9422	3.2296	3.8073	1.9066	0.0095	0.0623	0.0042
1C-1_89	16.9433	5.6518	0.1131	0.0278	10.0374	9.0639	0.0120	0.0000	0.0000	0.0000	0.0694	0.0466
4B-11_87	13.4186	4.1129	2.2976	1.1415	7.3132	6.0411	2.2094	0.6155	0.1086	0.0000	0.0402	0.0025
4B-2_87	9.6710	2.9120	1.5579	0.7754	4.9499	4.0177	1.4594	0.3556	0.0442	0.0000	0.0245	0.0000
1B-8_89	27.8055	9.5000	0.1535	0.0507	18.1137	16.8957	0.0101	0.0000	0.0000	0.0000	0.0961	0.0665
1A-5_87	20.9127	7.3518	0.2084	0.0734	13.2426	11.8801	0.0189	0.0000	0.0050	0.0000	0.0760	0.0626
2B-10_89	9.5775	2.9032	1.7106	3.0422	4.7529	4.3116	3.5466	3.0602	1.8304	0.1388	0.0505	0.0096
1A-8_87	26.9861	9.6468	0.2268	0.0765	18.2821	16.7485	0.0250	0.0000	0.0000	0.0000	0.0649	0.0480
3B-18_87	0.0420	0.0516	0.4694	2.1393	3.3399	7.1886	6.5718	16.6913	11.3784	0.4069	0.8920	0.2445
2B-7_87	11.0683	3.3365	2.0450	2.2338	6.0758	5.8461	2.7955	3.2752	1.6151	0.0000	0.0480	0.0020
3C-1_89	7.5144	2.2183	1.0964	1.8767	2.9672	2.7403	2.1449	1.8267	0.9646	0.0168	0.0416	0.0019
1C-6_89	24.6781	8.4042	0.1221	0.0079	16.0406	15.1031	0.0000	0.0000	0.0000	0.0000	0.0724	0.0467
3C-8_87	10.3891	3.0921	1.9431	2.0333	5.0453	4.7546	2.4357	2.6802	1.3094	0.0045	0.0784	0.0023
2B-11_87	13.7741	4.2562	2.6119	2.9374	8.1883	7.9384	3.7003	4.4261	2.2329	0.0094	0.0622	0.0112

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1A-14_89	36.7042	13.7914	0.2667	0.0900	32.3531	31.7889	0.0360	0.0000	0.0000	0.0000	0.1907	0.1618
3A-13_89	15.6530	4.9893	2.8026	5.1027	8.2293	7.9857	6.1877	5.6918	3.7174	0.3349	0.1180	0.0339
2C-3_89	7.8904	2.3764	1.1502	2.3097	3.9219	3.6039	2.7830	2.5343	1.2291	0.0000	0.0194	0.0000
4B-10_87	12.8642	3.9348	2.1674	1.0783	6.9061	5.6724	2.0792	0.5707	0.1099	0.0000	0.0508	0.0053
4B-11_87	13.3890	4.1100	2.2905	1.1631	7.2973	6.0233	2.2088	0.6046	0.1247	0.0000	0.0323	0.0022
1A-3_87	16.8937	5.8190	0.1794	0.0597	9.8105	8.6548	0.0142	0.0000	0.0069	0.0000	0.0791	0.0480
4C-18_87	1.5403	1.2115	2.9153	3.6587	17.5530	23.2783	10.8228	5.1157	2.5309	0.1785	0.4105	0.2238
3A-16_89	10.9679	4.4641	4.0868	9.0790	13.0100	14.1423	12.1729	12.1814	7.7638	0.6248	0.2697	0.0932
4B-5_87	10.3592	3.1282	1.6645	0.8352	5.3067	4.3117	1.5681	0.3865	0.0504	0.0000	0.0239	0.0000
3A-7_89	10.0948	3.0437	1.5035	2.6829	4.2857	4.0693	3.1430	2.7746	1.7612	0.0876	0.0650	0.0084
1C-15_87	27.3947	11.6441	0.4177	0.1980	31.2893	30.8960	0.0528	0.0000	0.0198	0.0000	0.2227	0.2007
1B-12_87	30.2753	10.8395	0.3348	0.1368	20.4724	18.6576	0.0289	0.0000	0.0121	0.0000	0.1197	0.1181
2A-15_87	14.5795	5.1746	3.9425	4.9408	13.7167	14.2464	6.7348	8.6660	4.8246	0.0991	0.1192	0.0283
2C-10_89	9.9179	3.0025	1.7318	3.0978	4.9291	4.4669	3.6203	3.1521	1.9877	0.1037	0.0553	0.0115
3C-12_87	11.5384	3.4791	2.2365	2.4070	5.9567	5.6929	2.9437	3.2892	1.5632	0.0000	0.0978	0.0053
3A-12_87	12.5719	3.7829	2.4480	2.5875	6.4228	6.1142	3.1696	3.5217	1.6689	0.0053	0.0972	0.0057
2A-2_87	9.8346	2.9673	1.5917	1.8346	5.3681	5.2025	2.3795	2.9458	1.3363	0.0000	0.0289	0.0000
2B-7_89	8.4444	2.5212	1.4442	2.4644	3.8558	3.4229	2.7855	2.2613	1.2204	0.0494	0.0440	0.0050
1C-9_87	26.8416	9.5125	0.2466	0.0953	17.7857	16.0984	0.0272	0.0000	0.0000	0.0000	0.0972	0.0768

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2A-8_89	8.3327	2.4924	1.4304	2.4764	3.9079	3.4980	2.8419	2.3949	1.4087	0.0576	0.0371	0.0044
1A-7_89	23.9358	8.0732	0.1509	0.0372	14.6290	13.3980	0.0165	0.0000	0.0000	0.0000	0.0895	0.0559
3C-9_89	10.6226	3.2205	1.6096	2.8821	4.6246	4.4064	3.3375	2.9768	1.8433	0.0698	0.0633	0.0074
3A-1_87	7.2139	2.1123	1.2783	1.3541	3.3227	3.1185	1.6523	1.8396	0.7430	0.0000	0.0492	0.0000
1A-1_89	17.0129	5.6745	0.1083	0.0310	10.0722	9.1087	0.0127	0.0000	0.0000	0.0000	0.0628	0.0421
2C-16_87	10.7922	4.3298	4.0455	5.5880	15.1724	16.6438	8.0097	10.7346	5.7921	0.2582	0.1746	0.0549
2C-8_87	10.6437	3.2012	2.0113	2.1239	5.6664	5.4122	2.6455	3.0522	1.5298	0.0069	0.0504	0.0056
3B-12_87	12.6477	3.8119	2.4832	2.6470	6.5101	6.1601	3.1937	3.5329	1.6756	0.0054	0.1060	0.0032
1B-6_87	21.8501	7.6739	0.1880	0.0580	13.9145	12.5261	0.0171	0.0000	0.0000	0.0000	0.0731	0.0570
4B-6_87	11.0022	3.3232	1.7804	0.8828	5.6564	4.6163	1.6794	0.4155	0.0612	0.0000	0.0269	0.0000
2B-16_89	5.1210	2.5004	3.7272	9.5405	12.4838	14.2325	13.7008	14.3138	8.9037	0.6699	0.2238	0.1040
1B-8_89	28.7366	9.8702	0.1608	0.0573	19.0193	17.8353	0.0195	0.0000	0.0000	0.0000	0.0991	0.0808
3C-4_87	8.9813	2.6389	1.6193	1.6958	4.2353	3.9459	2.0986	2.3332	1.0614	0.0000	0.0712	0.0019
3B-5_89	8.4169	2.5065	1.2410	2.1084	3.3991	3.1873	2.4413	2.0809	1.1757	0.0338	0.0561	0.0085
2C-18_87	0.2812	0.3192	1.4290	4.7926	10.3625	18.1174	11.2016	23.9355	15.8166	0.6544	0.3845	0.1551
4C-4_87	10.1678	3.0676	1.6574	0.8186	5.2111	4.2200	1.5737	0.3714	0.0483	0.0000	0.0287	0.0000
1B-13_87	32.6334	12.1383	0.4033	0.1741	25.0227	23.2681	0.0407	0.0000	0.0000	0.0000	0.1484	0.1285
3C-19_87	0.0308	0.0333	0.2080	1.3041	2.0370	5.0639	5.2951	17.7396	14.5476	0.5445	1.1929	0.3490
2B-6_87	11.1161	3.3511	1.9210	2.1623	6.1792	5.9909	2.8104	3.5244	1.8014	0.0000	0.0347	0.0000

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2A-12_89	11.8839	3.6631	2.2040	3.9409	6.2863	5.7039	4.6145	4.0352	2.5319	0.2194	0.0624	0.0164
2C-10_87	13.0478	3.9798	2.3211	2.5999	7.5405	7.3576	3.4117	4.1490	2.0666	0.0000	0.0507	0.0000
4B-16_87	2.2758	1.5142	3.0673	3.6244	17.7675	22.5909	10.4704	4.8443	2.4038	0.2244	0.4103	0.2292
4C-14_87	18.4134	6.0456	3.8598	2.0903	12.7745	10.9429	4.1040	1.2766	0.3363	0.0045	0.0775	0.0232
3B-10_89	11.6090	3.5295	1.7251	3.1809	5.1718	4.9523	3.7628	3.4470	2.2101	0.1174	0.0684	0.0108
1A-7_89	25.7914	8.8123	0.1595	0.0438	16.9758	15.9657	0.0243	0.0000	0.0000	0.0000	0.0842	0.0586
3C-10_87	11.1293	3.3112	2.0499	2.1799	5.4963	5.2032	2.6897	2.9545	1.4314	0.0070	0.0857	0.0026
2B-13_87	16.3939	5.3937	3.4576	4.2416	12.5119	12.8606	5.7891	7.5765	4.4056	0.0101	0.0847	0.0077
1A-12_87	32.1222	11.7096	0.3189	0.1502	23.0509	21.3406	0.0313	0.0000	0.0274	0.0000	0.1298	0.0939
1C-12_87	23.1668	11.3648	0.3385	0.1477	21.7716	19.9508	0.0349	0.0000	0.0000	0.0000	0.1249	0.1029
2C-16_89	7.5183	3.2979	3.9407	9.1794	12.8595	13.8233	12.5694	12.6103	7.8825	0.6243	0.1860	0.0873
2B-19_87	0.0000	0.0000	0.1323	1.3011	1.8293	5.8410	6.6267	27.4375	24.5740	1.0076	0.7144	0.3065
2A-6_89	8.8304	2.6686	1.5065	2.6687	4.3106	3.8959	3.1038	2.7252	1.7099	0.0888	0.0503	0.0070
1C-6_87	23.2555	8.2221	0.1929	0.0598	15.1063	13.7262	0.0176	0.0000	0.0000	0.0000	0.0616	0.0419
1B-14_89	34.3628	13.0218	0.2888	0.1495	30.8182	29.8680	0.0377	0.0000	0.0090	0.0000	0.1919	0.1849
1C-16_87	19.1089	9.4310	0.3729	0.2282	34.7715	37.1203	0.0649	0.0000	0.0067	0.0000	0.2930	0.2598
1A-17_89	21.0121	9.9617	0.2954	0.1999	36.9162	39.6577	0.0525	0.0000	0.0000	0.0000	0.3454	0.2919
1B-18_89	1.4499	0.8308	0.0191	0.0240	6.6188	15.2652	0.0184	0.0420	0.0142	0.0208	3.7870	3.6715
3A-15_89	16.5054	5.8214	3.8878	7.7128	12.1507	12.4048	9.8480	9.3470	6.0730	0.5187	0.1871	0.0686

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1A-10_89	29.1836	10.0041	0.1907	0.0757	18.9325	17.4622	0.0222	0.0000	0.0000	0.0000	0.1146	0.0843
2A-17_89	2.5261	1.5075	3.2181	9.7303	12.0501	14.9550	15.3173	17.2724	11.2342	0.8767	0.2689	0.1281
2C-4_89	7.1310	2.1379	1.2089	2.1560	3.3935	3.0570	2.5062	2.1717	1.3248	0.0448	0.0364	0.0054
2C-2_87	8.8543	2.6540	1.0996	1.6326	4.8690	4.7575	1.9812	2.5088	0.9475	0.0000	0.0164	0.0000
1B-7_89	25.1491	8.4645	0.1777	0.0710	15.2347	13.7460	0.0147	0.0000	0.0000	0.0000	0.1133	0.0825
3B-3_89	8.4098	2.5086	1.3536	2.1799	3.4369	3.2169	2.4644	2.1246	1.1359	0.0107	0.0488	0.0067
2B-15_87	12.5252	4.8499	4.2940	5.9411	16.0680	17.6235	8.5267	11.9215	6.9363	0.1720	0.1634	0.0358
2A-2_89	7.1900	2.1538	1.2089	2.2128	3.4294	3.0906	2.5926	2.2982	1.4352	0.0720	0.0389	0.0033
1C-6_89	26.1061	8.9327	0.1398	0.0547	17.0353	15.9809	0.0197	0.0000	0.0000	0.0000	0.0900	0.0598
3B-2_89	8.1787	2.4288	1.1834	2.1192	3.3248	3.1293	2.4685	2.1765	1.3040	0.0252	0.0509	0.0021
2C-18_89	0.0166	0.0265	0.5946	4.2176	3.1341	6.7004	12.3105	24.7146	21.0343	1.5984	0.5809	0.2895
4B-11_87	13.4721	4.1341	2.2911	1.1492	7.3419	6.0529	2.2024	0.6363	0.1220	0.0000	0.0372	0.0023
2A-3_89	7.3120	2.2030	1.1648	2.1672	3.5176	3.1865	2.5547	2.2779	1.3493	0.0300	0.0345	0.0000
4C-9_87	12.8490	3.8969	2.1196	1.0417	6.7180	5.5187	1.9940	0.5387	0.0757	0.0000	0.0321	0.0000
2C-3_87	9.9457	3.0128	1.4542	1.9702	5.7418	5.7095	2.4904	3.4105	1.3011	0.0000	0.0216	0.0000
1C-16_89	22.0077	10.4931	0.2125	0.1258	39.7565	43.6233	0.0443	0.0000	0.0000	0.0000	0.3130	0.3100
2A-14_87	16.8480	5.6230	3.8315	4.6897	13.2989	13.6392	6.2567	8.0917	4.4442	0.0117	0.1033	0.0118
3A-4_87	8.8196	2.5881	1.6106	1.6986	4.1404	3.8961	2.0642	2.2988	1.0542	0.0000	0.0678	0.0017
2C-6_87	10.9803	3.3338	1.8315	2.1796	6.2399	6.1150	2.8727	3.6703	1.7674	0.0000	0.0407	0.0000

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
4A-16_87	2.3880	5.8514	5.0477	3.2194	18.9163	18.3794	6.9893	2.3352	0.9695	0.0239	0.1669	0.0735
2A-16_89	8.2562	3.6543	4.1055	9.7981	14.4076	15.5235	13.4147	13.4376	8.5335	0.7033	0.1731	0.0734
2A-12_89	12.0411	3.7115	2.1776	3.9938	6.4357	5.8854	4.6960	4.1273	2.6606	0.2515	0.0669	0.0183
2A-13_89	15.2519	4.9961	2.8066	6.0550	9.9906	9.5523	7.3356	7.0588	4.7215	0.2798	0.0462	0.0000
1A-4_89	20.5723	6.8826	0.1425	0.0512	12.2835	11.0834	0.0149	0.0000	0.0000	0.0000	0.0821	0.0546
2C-3_89	7.8040	2.3447	1.1812	2.3526	3.8730	3.5633	2.7635	2.6611	1.4831	0.0307	0.0197	0.0000
2B-4_89	7.4718	2.2368	1.2357	2.2170	3.5839	3.2437	2.6058	2.2824	1.3618	0.0529	0.0374	0.0020
1B-18_87	9.6149	5.9392	0.3010	0.2425	34.8345	41.5678	0.0770	0.0033	0.0000	0.0000	0.4205	0.3962
1A-8_87	25.1175	8.8859	0.2517	0.1080	16.3088	9.0431	0.0247	0.0000	0.0056	0.0000	0.0833	0.0794
1B-16_87	25.1829	11.2696	0.3802	0.2198	33.9865	34.6318	0.0487	0.0000	0.0118	0.0000	0.2292	0.2076
1B-7_87	24.5973	8.7135	0.2114	0.0736	16.1538	14.7045	0.0208	0.0000	0.0000	0.0000	0.0727	0.0445
2A-8_87	11.5182	3.4844	2.1062	2.2958	6.3944	6.1654	2.9635	3.5832	1.8094	0.0000	0.0599	0.0000
2A-13_87	16.5350	5.3435	3.2536	4.0046	11.6833	11.8696	5.4674	7.0281	3.7905	0.0000	0.0698	0.0075
2B-4_89	7.4732	2.2424	1.1396	2.2688	3.6922	3.3754	2.6889	2.5197	1.4563	0.0000	0.0223	0.0000
2C-6_89	7.9418	2.3968	1.3147	2.4290	3.8602	3.5021	2.8593	2.5412	1.6161	0.0785	0.0394	0.0079
4C-13_87	12.1275	5.3060	3.1141	1.6281	10.1568	8.5433	3.1256	0.9402	0.1970	0.0000	0.0497	0.0070
2A-12_87	14.7189	4.5815	2.6674	3.0840	9.0988	8.9841	4.0470	5.1592	2.7980	0.0000	0.0625	0.0056
3B-10_87	11.5883	3.4578	2.1665	2.2645	5.7097	5.4086	2.8337	3.0858	1.4737	0.0094	0.0939	0.0053
4A-7_87	11.2250	3.3937	1.8602	0.9265	5.8280	4.7678	1.7742	0.4366	0.0538	0.0000	0.0466	0.0016

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
3B-18_87	0.0392	0.0543	0.4648	2.1360	3.3320	7.1999	6.5544	16.6254	11.3371	0.4068	0.8917	0.2551
3A-19_87	0.1497	0.1721	0.9925	3.3171	5.6603	10.0222	7.8771	15.5804	9.8521	0.3520	0.7452	0.1935
2C-3_87	10.2806	3.0972	1.5473	1.9723	5.8632	5.7597	2.5916	3.1624	1.4509	0.0000	0.0281	0.0000
1C-13_87	32.8954	12.5222	0.3684	0.1515	27.1808	25.6388	0.0379	0.0000	0.0000	0.0000	0.1536	0.1593
4A-4_87	10.2424	3.0851	1.6586	0.8139	5.2257	4.2689	1.5443	0.3682	0.0468	0.0000	0.0223	0.0000
4A-12_87	14.4830	4.4770	2.5195	1.3046	8.1197	6.7317	2.4996	0.7356	0.1465	0.0000	0.0361	0.0025
3A-4_89	8.2082	2.4537	1.2315	2.1105	3.3526	3.1343	2.4664	2.1312	1.2727	0.0353	0.0577	0.0059
3A-18_89	1.1701	0.8352	2.3246	8.1658	9.1468	13.0830	14.4077	18.0146	11.9344	0.8511	0.5014	0.2230
2C-7_89	7.5290	2.2516	1.2632	2.2505	3.4941	3.1303	2.5634	2.1514	1.2314	0.0319	0.0365	0.0044
3B-15_87	13.0080	4.6247	3.8646	4.7888	11.4618	11.8591	6.2346	7.2370	3.6365	0.0844	0.2401	0.0437
3A-7_87	10.3336	3.0468	1.9107	1.9680	4.9462	4.6734	2.4441	2.7094	1.3059	0.0000	0.0843	0.0048
1C-16_87	19.1484	9.4522	0.3673	0.2284	34.8640	37.2274	0.0623	0.0000	0.0000	0.0000	0.2953	0.2721
3A-2_87	8.4622	2.4877	1.5317	1.5843	3.9676	3.7094	1.9537	2.1717	0.9628	0.0000	0.0654	0.0000
1B-17_87	18.2096	9.1964	0.3704	0.2363	35.8368	38.8034	0.0669	0.0000	0.0070	0.0000	0.3040	0.2793
3A-19_87	0.1465	0.1694	0.9984	3.2903	5.6077	9.8866	7.7589	15.6244	9.8068	0.3490	0.7457	0.2023
1B-9_87	25.8284	9.0896	0.2567	0.1074	16.7899	15.2273	0.0235	0.0000	0.0000	0.0000	0.0986	0.0751
1C-17_89	9.8655	6.0488	0.1915	0.1830	37.6556	46.0700	0.0638	0.0000	0.0000	0.0000	0.5048	0.4715
2A-17_89	2.4350	1.4418	3.0907	9.1409	11.0686	13.6707	14.1631	15.4369	9.5861	0.7009	0.2543	0.1231
2A-2_87	9.6017	2.8839	1.6761	1.8485	5.1478	4.9373	2.3424	2.8106	1.3707	0.0000	0.0361	0.0000

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2A-16_87	9.5039	3.9517	3.8833	5.7081	15.0396	16.8318	8.2728	11.4136	6.5174	0.2346	0.1717	0.0512
4A-11_87	13.9712	4.2910	2.3861	1.2144	7.7004	6.3766	2.3309	0.6664	0.1314	0.0000	0.0366	0.0000
3A-11_89	11.5760	3.5325	1.8520	3.2678	5.2109	4.9667	3.8289	3.4196	2.1023	0.1463	0.0816	0.0146
1C-1_87	13.1610	4.5375	0.1330	0.0460	7.6253	6.6948	0.0125	0.0000	0.0000	0.0000	0.0557	0.0337
1C-5_87	19.8724	6.9719	0.1795	0.0621	12.4050	11.0388	0.0182	0.0000	0.0000	0.0000	0.0664	0.0574
2C-14_89	14.7638	4.9662	3.4215	6.4922	10.3936	9.8316	7.8247	7.0591	4.3859	0.3877	0.0841	0.0193
3A-3_87	8.7287	2.5623	1.5708	1.6491	4.0953	3.8067	2.0520	2.2862	1.0399	0.0000	0.0644	0.0000
3B-16_87	7.2286	3.1348	3.6007	5.2938	11.9640	13.5257	7.5456	9.5133	4.9518	0.1795	0.3497	0.0726
3A-8_89	9.3469	2.8235	1.3990	2.4805	4.0134	3.7934	2.9032	2.5521	1.6050	0.0972	0.0597	0.0095
2A-4_89	8.3203	2.5010	1.3000	2.4741	4.1244	3.7708	2.9489	2.6925	1.7177	0.0556	0.0311	0.0000
1A-9_89	27.5129	9.3331	0.2055	0.0740	17.1474	15.6198	0.0170	0.0000	0.0126	0.0000	0.1133	0.0915
1B-3_87	16.2156	5.5762	0.1699	0.0590	9.4235	8.3427	0.0166	0.0000	0.0039	0.0000	0.0724	0.0374
2C-14_89	14.5056	4.8646	3.5606	6.6049	10.1662	9.5590	7.9820	7.1845	4.4563	0.3582	0.0891	0.0254
1A-12_89	22.3659	11.0021	0.2646	0.1165	20.7807	19.0560	0.0250	0.0000	0.0000	0.0000	0.1508	0.1211
2C-15_87	14.3598	5.1734	4.0529	5.1115	14.2751	14.9847	6.9803	9.2890	5.1589	0.1515	0.1386	0.0362
2A-17_87	4.2281	2.2054	3.2402	5.7485	14.0086	17.3741	9.3454	14.1330	7.9102	0.3231	0.2295	0.0850
1C-5_89	20.9409	6.9603	0.1615	0.0630	12.1142	10.8597	0.0156	0.0000	0.0069	0.0000	0.0961	0.0633
2C-5_89	8.1460	2.4372	1.3825	2.4541	3.8888	3.5020	2.8560	2.4608	1.4735	0.0490	0.0362	0.0062
4C-16_87	16.0979	6.2561	5.2129	3.1547	18.9868	18.2590	6.8799	2.2479	0.8901	0.0148	0.1514	0.0641

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1A-17_89	20.8638	9.8919	0.2860	0.1943	36.7489	40.9382	0.0547	0.0000	0.0179	0.0000	0.3425	0.2950
3A-4_87	8.8563	2.6031	1.6340	1.6662	4.1663	3.9113	2.0892	2.2656	1.0785	0.0048	0.0705	0.0019
3B-5_87	9.3358	2.7400	1.6465	1.7612	4.4015	4.1456	2.1781	2.4323	1.1539	0.0000	0.0795	0.0000
3B-8_87	10.9697	3.2474	2.0293	2.1097	5.3298	5.0303	2.5647	2.8967	1.3667	0.0036	0.0931	0.0050
3B-3_87	8.7270	2.5591	1.5979	1.6604	4.1048	3.8562	2.0625	2.2836	1.0124	0.0000	0.0696	0.0020
1A-13_89	37.1009	13.4970	0.2525	0.0933	29.5491	28.5313	0.0335	0.0000	0.0000	0.0000	0.1628	0.1418
3B-4_89	8.7872	2.6221	1.2952	2.2350	3.5596	3.3324	2.5704	2.2245	1.2573	0.0138	0.0545	0.0055
3A-1_87	7.2420	2.1228	1.2689	1.3285	3.3473	3.0922	1.6481	1.8377	0.7641	0.0000	0.0517	0.0000
1B-12_89	23.4990	10.7681	0.2620	0.1098	20.3135	18.5872	0.0256	0.0000	0.0000	0.0000	0.1574	0.1217
1B-16_89	17.6708	8.8608	0.2773	0.1973	37.0292	41.4498	0.0590	0.0000	0.0000	0.0000	0.3811	0.3413
1C-12_87	33.3431	12.1807	0.3038	0.1174	24.2906	22.5831	0.0349	0.0000	0.0000	0.0000	0.1080	0.0854
3A-2_87	8.4878	2.4894	1.5652	1.6169	3.9798	3.7251	2.0003	2.2155	0.9721	0.0000	0.0657	0.0000
1C-13_89	35.5437	12.8526	0.3011	0.1336	27.5014	26.1220	0.0311	0.0000	0.0073	0.0000	0.1900	0.1618
1B-5_89	22.8124	7.6842	0.1575	0.0605	13.9846	12.7801	0.0151	0.0000	0.0000	0.0000	0.0910	0.0659
1B-5_89	22.3050	7.4979	0.1539	0.0562	13.5545	12.3366	0.0152	0.0000	0.0093	0.0000	0.0906	0.0649
2B-18_87	0.0991	0.1636	0.9675	4.1325	8.3862	16.5816	11.3751	27.9430	20.4515	0.9207	0.4507	0.1773
4C-1_87	8.4619	2.5419	1.3909	0.6809	4.2510	3.4790	1.2795	0.3074	0.0318	0.0000	0.0277	0.0000
1B-9_87	25.9352	9.1927	0.2457	0.1099	17.0091	15.4192	0.0238	0.0000	0.0072	0.0000	0.0939	0.0674
4A-1_87	8.9319	2.6781	1.4701	0.7038	4.5291	3.6676	1.3665	0.3216	0.0360	0.0000	0.0283	0.0000

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
3B-1_89	7.4746	2.2238	1.0896	1.9465	3.0217	2.8339	2.2410	1.9450	1.1082	0.0121	0.0503	0.0033
2C-4_89	7.1506	2.1241	1.1415	2.1146	3.3859	3.0518	2.4615	2.1717	1.2171	0.0247	0.0211	0.0000
1B-1_89	17.6314	5.9257	0.1065	0.0250	10.7389	9.8470	0.0117	0.0000	0.0000	0.0000	0.0557	0.0365
1C-2_89	19.5405	6.5135	0.1406	0.0621	11.5396	10.3581	0.0129	0.0000	0.0105	0.0000	0.0863	0.0591
4C-2_87	9.5761	2.8806	1.5351	0.7695	4.8733	3.9444	1.4263	0.3283	0.0428	0.0000	0.0234	0.0000
1C-13_89	36.6084	13.2997	0.3059	0.1485	28.7113	27.3490	0.0346	0.0000	0.0000	0.0000	0.1995	0.1646
3B-17_87	1.4824	0.9555	2.1294	4.7416	9.4192	13.0797	8.3464	12.9212	7.1564	0.2712	0.5209	0.1339
2B-9_87	12.4135	3.7707	2.3568	2.5472	7.0017	6.7305	3.2361	3.8306	1.9288	0.0133	0.0645	0.0066
1C-3_87	16.2570	5.5855	0.1671	0.0609	9.4273	8.1263	0.0133	0.0000	0.0105	0.0000	0.0739	0.0468
4B-9_87	12.1268	3.6764	1.9874	0.9989	6.3632	5.2285	1.8800	0.4782	0.0693	0.0000	0.0282	0.0000
3B-11_89	12.5513	3.8248	1.9657	3.4600	5.6311	5.3611	4.0860	3.6924	2.4009	0.1957	0.0785	0.0151
2C-7_89	7.5873	2.2621	1.2990	2.2517	3.5375	3.1651	2.5819	2.1763	1.2403	0.0453	0.0448	0.0053
1B-14_89	34.4869	13.1344	0.2653	0.1088	31.4342	30.7324	0.0390	0.0000	0.0443	0.0000	0.1998	0.1648
1A-4_87	17.8198	6.0628	0.1837	0.0681	10.3266	9.1202	0.0183	0.0000	0.0110	0.0000	0.0735	0.0479
2C-9_87	12.1004	3.6631	2.2133	2.4165	6.6732	6.4175	3.0445	3.5722	1.7746	0.0039	0.0597	0.0043
2B-9_89	8.9768	2.7006	1.5943	2.8156	4.3348	3.9041	3.2727	2.8069	1.6904	0.0873	0.0426	0.0069
2B-13_87	16.1740	5.3016	3.4230	4.0967	12.0253	12.1954	5.4481	6.8236	3.6370	0.0141	0.0844	0.0104
2B-16_89	5.0192	2.4428	3.6041	9.0943	11.9692	13.5443	13.0583	13.2979	7.9879	0.5674	0.2199	0.1007
1C-15_89	29.3651	11.8326	0.3092	0.1751	31.2640	31.1058	0.0390	0.0000	0.0131	0.0000	0.2507	0.2151

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1B-1_89	17.3377	5.8252	0.1068	0.0306	10.4483	9.5555	0.0097	0.0000	0.0000	0.0000	0.0736	0.0369
4B-15_87	6.6033	3.4932	4.3857	3.7250	20.5497	22.3163	9.1606	3.5498	1.6915	0.0810	0.2678	0.1334
4A-1_87	8.8854	2.6712	1.4729	0.7051	4.4939	3.6747	1.3744	0.3112	0.0296	0.0000	0.0274	0.0000
3C-3_87	9.0386	2.6532	1.6406	1.6859	4.2615	4.0213	2.1316	2.3772	1.0960	0.0051	0.0700	0.0022
1C-9_89	28.8407	9.8811	0.1742	0.0600	18.9422	17.7402	0.0179	0.0000	0.0000	0.0000	0.1115	0.0784
2A-7_89	8.7727	2.6450	1.4994	2.6926	4.3476	3.9560	3.2209	2.8836	1.8774	0.1066	0.0431	0.0038
3A-9_87	11.3251	3.3583	2.0557	2.1755	5.5184	5.2115	2.6801	2.9876	1.3871	0.0000	0.0843	0.0049
3B-12_89	12.9549	3.9793	2.0776	3.6946	6.0010	5.7478	4.3811	3.9445	2.5854	0.2366	0.0857	0.0213
3B-7_89	10.2230	3.0513	1.4928	2.6462	4.3050	4.0772	3.1034	2.7978	1.7332	0.0794	0.0594	0.0086
1C-14_89	34.5950	13.2822	0.2911	0.1281	32.1876	31.5589	0.0406	0.0000	0.0405	0.0000	0.2062	0.1820
3A-5_89	8.5364	2.5393	1.2727	2.1980	3.4354	3.1972	2.5172	2.1349	1.2106	0.0179	0.0608	0.0057
2A-1_87	7.6682	2.3010	1.1560	1.4684	4.1220	3.9744	1.8386	2.2768	0.8588	0.0000	0.0117	0.0000
3A-17_87	7.1363	3.0812	3.5682	5.1999	11.7812	13.2865	7.3772	9.3786	4.8546	0.1837	0.3395	0.0745
1A-19_89	4.6070	3.5423	0.1366	0.1938	36.2507	50.0845	0.0740	0.0043	0.0000	0.0000	0.7106	0.6543
3C-3_87	9.0075	2.6431	1.6565	1.7227	4.2529	4.0050	2.1403	2.3896	1.1113	0.0000	0.0707	0.0025
4B-4_87	10.2363	3.0811	1.6621	0.8145	5.2496	4.2544	1.5757	0.3924	0.0467	0.0000	0.0272	0.0000
4B-6_87	11.0930	3.3453	1.7670	0.8923	5.7066	4.6645	1.6552	0.4278	0.0506	0.0000	0.0238	0.0000
2B-2_89	7.5262	2.2464	1.1041	2.1965	3.6422	3.3309	2.6421	2.4026	1.3729	0.0381	0.0276	0.0000
4C-12_87	13.5617	4.1844	2.3500	1.1732	7.4428	6.1310	2.2581	0.5968	0.0838	0.0000	0.0346	0.0000

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
3C-8_89	9.7294	2.9222	1.4708	2.5936	4.1006	3.8716	3.0063	2.6518	1.5983	0.0597	0.0644	0.0077
4B-2_87	9.6610	2.9097	1.5542	0.7682	4.9337	3.9979	1.4617	0.3568	0.0421	0.0000	0.0289	0.0000
3A-7_89	10.2304	3.0736	1.5258	2.7220	4.3553	4.1439	3.1750	2.8460	1.7353	0.1045	0.0553	0.0098
2C-15_89	13.6944	4.9134	3.9110	7.8633	11.9816	11.6778	9.7410	8.9583	5.4516	0.4506	0.1180	0.0412
1B-13_89	37.7776	13.6673	0.3320	0.1442	29.5968	28.0760	0.0356	0.0000	0.0000	0.0000	0.1957	0.1593
2C-11_87	14.6938	4.5608	2.5255	3.0556	9.2160	9.2000	4.0423	5.2574	2.9082	0.0000	0.0495	0.0000
3B-16_87	7.2504	3.1463	3.6136	5.3106	12.0288	13.5933	7.5594	9.5519	4.9681	0.1715	0.3447	0.0763
4C-9_87	12.8408	3.8988	2.0913	1.0505	6.7545	5.5149	2.0041	0.5412	0.0749	0.0000	0.0283	0.0000
1C-14_87	30.0210	11.8081	0.4408	0.1846	27.5710	26.6116	0.0460	0.0000	0.0000	0.0000	0.1897	0.1908
2C-13_89	12.9453	4.1436	2.6209	4.9336	7.7994	7.2660	5.9355	5.3366	3.4363	0.3017	0.0482	0.0131
2C-14_87	14.9201	5.0619	3.6218	4.4856	12.3282	12.6716	5.9972	7.7693	4.2909	0.0789	0.1057	0.0216
1B-13_89	37.4814	13.7582	0.3019	0.1464	30.2246	28.9186	0.0318	0.0000	0.0000	0.0000	0.1876	0.1654
2A-10_87	12.6648	3.8568	2.3407	2.5874	7.1805	6.9351	3.2684	3.9231	1.9982	0.0000	0.0566	0.0044
3A-2_89	7.4958	2.2298	1.0925	1.9080	3.0236	2.8200	2.2085	1.8996	1.0666	0.0406	0.0547	0.0017
3B-3_87	8.7301	2.5635	1.6083	1.6554	4.1039	3.8644	2.0546	2.2628	1.0259	0.0048	0.0689	0.0020
1A-5_87	20.4233	7.1348	0.2133	0.0791	12.7092	11.4408	0.0184	0.0000	0.0044	0.0000	0.0750	0.0578
1B-4_87	17.2511	5.9208	0.1753	0.0579	10.0293	8.8740	0.0133	0.0000	0.0000	0.0000	0.0689	0.0496
4B-16_87	2.3016	1.5408	3.0731	3.6303	18.1361	23.3039	10.3954	4.8361	2.4743	0.2012	0.4059	0.2226
2B-8_87	12.6449	3.8663	2.2225	2.5032	7.3452	7.1711	3.2369	3.9647	2.0186	0.0000	0.0550	0.0000

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
3B-12_87	12.7834	3.8607	2.4661	2.6402	6.5919	6.2628	3.2488	3.5714	1.7224	0.0050	0.0932	0.0027
3A-5_87	9.4007	2.7658	1.6576	1.7560	4.4454	4.1863	2.1689	2.4318	1.1288	0.0000	0.0669	0.0022
4C-10_87	12.9598	3.9550	2.1795	1.0951	6.8816	5.6536	2.0777	0.5354	0.0768	0.0000	0.0244	0.0000
4A-9_87	12.1806	3.7155	2.0517	1.0431	6.5400	5.3937	1.9782	0.5441	0.1010	0.0000	0.0353	0.0040
3B-8_87	10.9729	3.2430	2.0079	2.1115	5.3333	5.0451	2.6028	2.8741	1.3592	0.0046	0.0884	0.0020
2B-4_89	7.8646	2.3606	1.1788	2.3781	3.9458	3.6286	2.8840	2.6984	1.6322	0.0237	0.0301	0.0000
4B-13_87	12.4732	5.5078	3.2748	1.7160	10.6245	8.9683	3.2934	0.9836	0.2210	0.0000	0.0580	0.0083
3C-17_89	8.0841	3.5847	3.8707	8.9975	12.6405	14.3466	12.5107	12.6817	7.9297	0.6014	0.3007	0.1106
1C-10_89	30.2150	10.3169	0.2206	0.0985	19.4686	17.8932	0.0192	0.0000	0.0000	0.0000	0.1299	0.0917
3C-8_89	9.7846	2.9236	1.4665	2.5765	4.1006	3.8518	3.0022	2.6227	1.5915	0.0686	0.0607	0.0128
1A-13_89	36.0422	13.1484	0.2192	0.0643	28.9393	28.3233	0.0282	0.0000	0.0325	0.0000	0.1581	0.1362
1C-8_87	26.5338	9.4906	0.2189	0.0702	18.2835	17.0113	0.0225	0.0000	0.0000	0.0000	0.0713	0.0661
2C-5_87	10.7325	3.2311	1.7838	2.0716	5.9602	5.7901	2.6760	3.3398	1.6531	0.0000	0.0282	0.0000
2C-7_87	10.9908	3.3220	1.9147	2.2064	6.1387	5.9514	2.9406	3.5673	1.7829	0.0000	0.0334	0.0000
2A-6_87	10.8961	3.3031	1.8519	2.1892	6.1802	6.0073	2.8146	3.4590	1.7989	0.0000	0.0359	0.0000
4A-5_87	10.5029	3.1616	1.6964	0.8500	5.3729	4.3971	1.5861	0.3769	0.0571	0.0000	0.0312	0.0019
2C-12_89	12.0351	3.7340	2.1822	3.8993	6.5159	5.9943	4.6449	4.1787	2.7074	0.2575	0.0618	0.0094
1C-9_87	27.2936	9.7868	0.1941	0.0658	18.7207	17.3386	0.0251	0.0000	0.0000	0.0000	0.0553	0.0427
1C-18_87	2.1143	1.9399	0.1332	0.1960	27.0628	40.2002	0.0836	0.0311	0.0000	0.0038	0.7538	0.6741

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1B-4_87	17.1507	5.8910	0.1801	0.0661	9.9515	8.8012	0.0176	0.0000	0.0000	0.0000	0.0664	0.0506
3C-17_87	3.2597	1.7537	2.8311	5.1453	10.9186	13.7145	8.1542	11.6236	6.2649	0.2411	0.4544	0.1140
3C-13_87	14.7599	4.6184	3.1124	3.5102	8.6080	8.3658	4.3314	4.8005	2.3517	0.0178	0.1493	0.0191
4C-2_87	9.4784	2.8417	1.5364	0.7628	4.8183	3.9074	1.4283	0.3418	0.0396	0.0000	0.0308	0.0000
1B-10_87	31.3123	11.3414	0.2579	0.1081	22.5199	20.9052	0.0331	0.0000	0.0000	0.0000	0.1021	0.0662
1A-14_89	32.9878	12.1902	0.2481	0.0745	27.2695	26.4004	0.0282	0.0000	0.0446	0.0000	0.1874	0.1533
2A-11_89	11.1558	3.4162	2.0384	3.6263	5.7641	5.2203	4.2515	3.7728	2.3965	0.1613	0.0685	0.0113
3B-1_87	7.3464	2.1612	1.3535	1.3862	3.4212	3.1738	1.7207	1.8990	0.8047	0.0000	0.0559	0.0000
2B-16_87	6.3877	3.1561	3.7419	6.5816	17.9661	22.1357	10.6280	16.6013	10.1784	0.4842	0.2181	0.0783
3A-4_89	8.2776	2.4699	1.2517	2.1620	3.3758	3.1735	2.4916	2.1566	1.1882	0.0136	0.0536	0.0066
2A-3_87	9.8598	2.9649	1.6734	1.9177	5.3556	5.1927	2.4418	2.9047	1.4331	0.0000	0.0323	0.0000
3A-8_87	11.0452	3.2668	2.0456	2.1233	5.3093	5.0048	2.6267	2.8872	1.3814	0.0000	0.0935	0.0050
1A-8_87	26.3373	9.3863	0.2151	0.0721	17.6320	16.0902	0.0222	0.0000	0.0099	0.0000	0.0756	0.0668
2B-1_89	6.9394	2.0832	1.0867	2.1013	3.3501	3.0443	2.4865	2.3099	1.3439	0.0162	0.0188	0.0000
1B-4_89	21.5298	7.2874	0.1423	0.0389	13.3589	12.3196	0.0174	0.0000	0.0000	0.0000	0.0855	0.0493
3A-6_89	9.4567	2.8188	1.4095	2.4227	3.8980	3.6424	2.7981	2.4041	1.3939	0.0794	0.0579	0.0074
3B-3_89	8.0944	2.4006	1.1860	2.0428	3.2011	2.9813	2.3143	1.9525	1.0944	0.0144	0.0519	0.0062
2B-14_89	14.6353	5.0065	3.6157	7.0840	10.9732	10.4627	8.6455	7.8497	4.7508	0.4003	0.1018	0.0303
1C-7_89	27.0255	9.2962	0.1374	0.0379	18.0009	17.1152	0.0168	0.0000	0.0000	0.0000	0.0922	0.0740

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1C-13_87	33.5257	12.7637	0.3712	0.1843	27.8259	26.4154	0.0369	0.0000	0.0166	0.0000	0.1511	0.1499
1A-5_87	21.2984	7.5093	0.1843	0.0584	13.5917	12.2363	0.0193	0.0000	0.0000	0.0000	0.0711	0.0562
3A-10_87	11.4767	3.4046	2.1426	2.2320	5.6413	5.3426	2.7267	3.0340	1.4528	0.0048	0.0924	0.0047
3C-14_87	14.2445	4.6539	3.3741	3.8533	9.3255	9.1953	4.8313	5.4257	2.6502	0.0184	0.1669	0.0174
2C-2_87	8.7766	2.6393	1.3694	1.7364	4.8240	4.7131	2.1972	2.8139	1.2334	0.0000	0.0230	0.0000
4A-11_87	13.7948	4.2595	2.4035	1.2117	7.6323	6.3179	2.3324	0.6812	0.1334	0.0000	0.0442	0.0045
2C-17_89	1.5841	1.0298	2.6779	8.6477	9.9694	12.8412	14.2879	16.7045	10.7737	0.7855	0.2942	0.1375
2C-13_89	13.4516	4.3208	2.6263	4.9744	8.2228	7.6554	6.0213	5.4760	3.5296	0.2607	0.0465	0.0070
3C-19_89	0.1046	0.1347	1.1139	6.0608	5.4530	10.1401	14.3631	23.2629	17.2727	1.2653	0.7017	0.2914
1C-15_89	30.2865	12.2103	0.3001	0.1639	32.5243	32.6345	0.0392	0.0000	0.0000	0.0000	0.2501	0.2215
1C-5_87	19.5235	6.8388	0.1937	0.0734	11.9732	10.6690	0.0177	0.0000	0.0036	0.0000	0.0734	0.0562
1B-15_89	28.8847	12.1397	0.3010	0.1715	35.1365	35.9632	0.0447	0.0000	0.0000	0.0000	0.2616	0.2262
2A-1_87	7.5288	2.2563	1.2493	1.4334	3.9679	3.8098	1.8152	2.2049	0.9242	0.0000	0.0175	0.0000
2A-15_87	15.8861	5.6682	4.1434	5.3795	15.8843	16.8858	7.5033	10.0988	5.7885	0.0606	0.1157	0.0255
1A-18_87	3.7438	2.8134	0.1840	0.1956	24.1647	31.6618	0.0721	0.0185	0.0000	0.0000	0.5346	0.5184
1C-16_89	22.6111	10.8909	0.2194	0.1551	42.8106	47.4665	0.0440	0.0000	0.0000	0.0000	0.3391	0.3121
1C-4_89	21.9939	7.4219	0.1248	0.0299	13.6619	12.5923	0.0166	0.0000	0.0000	0.0000	0.0667	0.0454
1B-8_87	26.7568	9.5695	0.2279	0.0570	18.3239	16.8683	0.0229	0.0000	0.0000	0.0000	0.0585	0.0490
2C-8_87	10.8801	3.2951	1.9911	2.1314	5.9457	5.6803	2.7188	3.1460	1.5966	0.0000	0.0555	0.0022

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1A-14_89	33.5459	12.3960	0.3089	0.1401	27.4226	26.4313	0.0329	0.0000	0.0000	0.0000	0.2039	0.1617
2C-5_87	10.7657	3.2701	1.7465	2.0968	6.1358	6.0186	2.7311	3.5779	1.6568	0.0000	0.0290	0.0000
3B-12_89	12.7803	3.8998	2.0418	3.5014	5.6538	5.3014	4.0589	3.5024	2.0190	0.1623	0.0952	0.0194
3A-16_89	10.9698	4.4645	4.0248	8.8374	12.9341	13.9606	11.8576	11.8263	7.4723	0.5913	0.2696	0.1091
3A-12_89	13.0211	3.9951	2.0957	3.7213	5.9456	5.6693	4.3905	3.8865	2.3606	0.2137	0.0879	0.0205
1C-19_87	0.3003	0.3292	0.0000	0.0602	13.8069	32.0384	0.0550	0.0135	0.0000	0.0070	1.7833	1.7929
3B-17_89	2.5046	1.5070	2.9699	8.9687	10.8675	14.2933	14.4987	16.7999	10.8732	0.7875	0.4632	0.1765
3B-14_87	14.5522	4.8209	3.7392	4.2088	10.2074	10.1075	5.2645	5.9494	3.0128	0.0789	0.2142	0.0388
2C-12_87	14.5895	4.5077	2.7897	3.1321	8.8502	8.6474	3.9800	4.8811	2.5515	0.0165	0.0769	0.0125
3A-11_87	12.3258	3.6915	2.3334	2.5232	6.2119	5.9040	3.0919	3.4088	1.6127	0.0051	0.1041	0.0050
1C-10_87	29.4871	10.6213	0.2510	0.1134	20.3961	18.7990	0.0324	0.0000	0.0000	0.0000	0.0997	0.0689
2C-19_87	0.0427	0.0780	0.7674	3.3251	5.9342	12.1926	9.5008	23.4571	16.1921	0.6352	0.4601	0.1933
1B-9_87	26.6198	9.4747	0.2509	0.0816	17.7365	16.1280	0.0212	0.0000	0.0000	0.0000	0.0777	0.0593
2C-17_87	4.7772	2.4955	3.4166	6.3717	16.0633	20.1592	10.2636	16.0593	9.4670	0.4511	0.2385	0.0834
1C-18_89	1.2143	1.3400	0.0634	0.1733	28.9293	47.8253	0.0785	0.0432	0.0029	0.0040	1.0779	0.9995
4B-15_87	6.6330	3.5099	4.3752	3.7306	20.6495	18.3666	9.1747	3.5621	1.7263	0.0689	0.2680	0.1354
1C-1_89	16.1843	5.3683	0.1166	0.0415	9.2400	8.2603	0.0116	0.0000	0.0000	0.0000	0.0783	0.0422
2B-3_87	9.9258	3.0013	1.3915	1.9321	5.6815	5.6508	2.5386	3.1440	1.2617	0.0000	0.0159	0.0000
2B-9_87	12.9584	3.9614	2.3151	2.6400	7.6592	7.5300	3.4570	4.2667	2.1788	0.0000	0.0521	0.0000

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
4C-11_87	13.3329	4.0813	2.2748	1.1364	7.1869	5.9124	2.1651	0.5924	0.0685	0.0000	0.0332	0.0000
3A-6_89	9.5334	2.8610	1.4108	2.4976	3.9781	3.7422	2.8903	2.5361	1.5561	0.0758	0.0629	0.0099
1B-17_89	9.1769	5.8677	0.1494	0.1494	40.6183	51.0380	0.0602	0.0000	0.0000	0.0000	0.5412	0.4852
1B-13_89	34.6250	12.4387	0.3292	0.1401	26.1324	24.5983	0.0349	0.0000	0.0000	0.0000	0.1973	0.1614
3B-14_87	14.9187	4.9431	3.6943	4.2872	10.4154	10.3673	5.3967	6.1289	3.0556	0.0400	0.1981	0.0251
2C-13_87	15.2432	4.8965	3.2235	3.7301	10.5007	10.5441	5.0520	6.2558	3.2546	0.0145	0.0782	0.0066
3A-13_87	14.5241	4.5235	3.0442	3.3915	8.3883	8.1031	4.1897	4.6940	2.2935	0.0186	0.1394	0.0110
3A-12_89	13.1608	4.0458	2.1063	3.7295	6.0292	5.7694	4.4022	3.9083	2.4640	0.2126	0.0931	0.0207
3C-7_89	9.6065	2.8936	1.4296	2.5209	4.0489	3.8121	2.9208	2.5627	1.6136	0.0886	0.0591	0.0094
1B-18_89	1.4967	0.8773	0.0194	0.0058	7.3515	17.4275	0.0201	0.0418	0.0187	0.0167	3.8319	3.8645
3A-5_89	8.6256	2.5673	1.3089	2.2394	3.5030	3.2701	2.5795	2.2106	1.2627	0.0235	0.0618	0.0037
1A-18_89	12.2288	6.8208	0.2475	0.2203	35.2549	40.7167	0.0613	0.0119	0.0000	0.0000	0.4524	0.4078
2A-3_89	7.4355	2.2273	1.1647	2.2775	3.6456	3.3211	2.6845	2.5279	1.4760	0.0199	0.0190	0.0000
2A-10_89	10.5678	3.2220	1.9235	3.3342	5.3321	4.8720	3.9097	3.4821	2.2702	0.1172	0.0555	0.0103
2A-2_87	9.9656	3.0224	1.6246	1.9926	5.5985	5.4653	2.5303	3.1728	1.4364	0.0000	0.0185	0.0000
2A-1_87	7.5318	2.2528	1.0817	1.3967	4.0904	3.9412	1.7726	2.1401	0.7924	0.0000	0.0129	0.0000
3A-15_89	15.7097	5.5060	3.8110	7.3546	11.2488	11.3283	9.1571	8.6583	5.3868	0.4303	0.1909	0.0644
1C-18_87	2.1803	2.0180	0.1328	0.1851	28.6866	48.0253	0.0972	0.0217	0.0000	0.0023	0.7721	0.7015
1C-6_87	22.5681	7.9631	0.1870	0.0503	14.4347	13.0135	0.0211	0.0000	0.0000	0.0000	0.0754	0.0423

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1A-11_87	31.5911	11.4881	0.2871	0.1256	22.6454	20.8724	0.0312	0.0000	0.0000	0.0000	0.1123	0.0976
1C-2_89	19.4002	6.4743	0.1396	0.0513	11.4337	10.2443	0.0129	0.0026	0.0053	0.0000	0.0859	0.0569
4A-6_87	10.8994	3.2867	1.7958	0.8824	5.6374	4.6222	1.7017	0.4247	0.0679	0.0000	0.0368	0.0018
2C-7_89	7.7316	2.3233	1.3249	2.3125	3.6898	3.3161	2.7044	2.3346	1.4144	0.0495	0.0311	0.0064
2A-15_87	15.0715	5.3624	4.0230	5.1233	14.5504	15.3001	7.1560	9.3466	5.2191	0.0658	0.1181	0.0259
1A-19_87	0.3751	0.5605	0.0286	0.1249	20.1294	37.6398	0.0758	0.0217	0.0000	0.0000	1.1574	1.0896
2B-18_89	0.0270	0.0452	0.7816	5.1618	3.8931	7.9136	13.8413	25.1214	20.0420	1.5056	0.5211	0.2647
1C-15_87	28.1730	11.9987	0.4127	0.2129	32.6029	32.3342	0.0562	0.0000	0.0268	0.0000	0.2270	0.2035
1A-17_87	12.9095	7.2227	0.2916	0.2208	34.6583	39.3292	0.0621	0.0000	0.0197	0.0000	0.3630	0.3452
3C-18_87	0.3973	0.3467	1.2754	3.6664	6.8896	11.1886	8.0754	14.8778	9.0255	0.3211	0.6776	0.1893
4C-10_87	12.9305	3.9337	2.1729	1.1033	6.8746	5.6307	2.0729	0.5386	0.0784	0.0000	0.0335	0.0000
2C-14_87	15.0718	5.1551	3.6028	4.4553	12.4768	12.7782	5.8938	7.5992	4.2044	0.0517	0.1040	0.0137
1B-6_87	21.5036	7.5457	0.2041	0.0749	13.5217	12.0555	0.0193	0.0000	0.0076	0.0000	0.0753	0.0493
3B-18_89	0.1933	0.2032	1.2574	6.3803	6.0094	10.7263	14.6061	23.8301	18.3468	1.3967	0.7036	0.2932
2A-1_89	6.6713	1.9860	1.0951	2.0380	3.1278	2.8083	2.3554	2.1152	1.2701	0.0308	0.0271	0.0000
1A-3_87	16.8761	5.8139	0.1793	0.0623	9.7926	8.6431	0.0138	0.0000	0.0000	0.0000	0.0735	0.0476
3C-9_87	10.5840	3.1421	1.9676	2.0673	5.1742	4.8976	2.5714	2.8333	1.3329	0.0000	0.0882	0.0027
1C-17_89	9.7610	5.9482	0.2109	0.2044	36.7961	44.7854	0.0673	0.0000	0.0000	0.0000	0.5053	0.4618
4B-7_87	11.5109	3.4841	1.8766	0.9413	6.0042	4.9338	1.7843	0.4680	0.0648	0.0000	0.0235	0.0000

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
3C-4_87	9.0082	2.6471	1.6345	1.6680	4.2531	3.9697	2.1140	2.3628	1.0585	0.0000	0.0701	0.0021
4B-3_87	9.8163	2.9521	1.5968	0.7922	4.9954	4.0421	1.4777	0.3648	0.0366	0.0000	0.0180	0.0000
1C-5_87	20.1802	7.0670	0.1756	0.0575	12.6055	11.3055	0.0155	0.0000	0.0000	0.0000	0.0704	0.0578
3C-12_89	12.1159	3.7133	1.9420	3.4423	5.5408	5.3102	4.0697	3.6251	2.3377	0.1862	0.0803	0.0174
3B-14_89	16.5604	5.5102	3.4024	6.4295	9.9744	9.8230	7.8676	7.2848	4.6442	0.3998	0.1620	0.0561
2A-18_89	0.2267	0.2419	1.6468	7.7545	7.3945	12.0503	16.1552	23.2370	16.5535	1.2688	0.3997	0.2043
3C-2_89	7.5093	2.2224	1.0915	1.9740	3.0413	2.8458	2.2544	1.9844	1.1222	0.0142	0.0491	0.0000
2C-10_87	12.5411	3.8402	2.2638	2.5387	7.1722	6.9680	3.3036	3.9656	2.0228	0.0000	0.0472	0.0000
1A-9_87	27.8339	9.9598	0.2248	0.0622	18.9226	17.5084	0.0291	0.0000	0.0000	0.0000	0.0751	0.0652
2B-7_87	12.4900	3.8291	2.1442	2.5226	7.6466	7.6672	3.3426	4.3005	2.1548	0.0000	0.0505	0.0000
3A-2_89	7.4805	2.2271	1.0939	1.9053	3.0035	2.8016	2.1909	1.8983	1.0796	0.0160	0.0457	0.0040
4C-10_87	12.9769	3.9611	2.1782	1.0899	6.8890	5.6581	2.0778	0.5609	0.0754	0.0000	0.0303	0.0000
1B-10_87	30.0946	10.8745	0.2677	0.1008	21.3860	19.8243	0.0248	0.0000	0.0000	0.0000	0.0961	0.0633
3B-2_87	8.1501	2.3925	1.4713	1.5325	3.8132	3.5828	1.8942	2.0989	0.9412	0.0000	0.0641	0.0000
2A-7_89	8.6483	2.6117	1.4945	2.6358	4.2407	3.8462	3.0916	2.7697	1.8012	0.1118	0.0438	0.0078
1A-6_87	22.7577	8.0521	0.1964	0.0704	14.7535	13.3441	0.0237	0.0000	0.0076	0.0000	0.0586	0.0526
3B-9_87	11.7093	3.4732	2.1683	2.2722	5.6785	5.3532	2.7799	3.0848	1.4612	0.0049	0.0923	0.0029
2C-5_87	10.2534	3.0768	1.7668	1.9764	5.5777	5.3617	2.5469	3.0533	1.5777	0.0000	0.0501	0.0000
1A-5_89	21.9378	7.3412	0.1514	0.0500	13.2418	11.9799	0.0148	0.0000	0.0049	0.0000	0.0970	0.0630

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2B-11_89	10.6170	3.2635	1.9338	3.4827	5.5805	5.0917	4.1177	3.6236	2.3023	0.2033	0.0539	0.0149
3C-15_89	17.2406	5.9202	3.7293	7.2796	11.6495	11.8111	9.1554	8.7174	5.7576	0.5230	0.1655	0.0530
1C-7_89	25.6279	8.6568	0.1571	0.0644	16.0043	14.7103	0.0150	0.0000	0.0000	0.0000	0.1019	0.0642
2C-6_87	11.1445	3.3676	1.8864	2.1745	6.2735	6.0792	2.7875	3.4821	1.7432	0.0000	0.0461	0.0000
4A-4_87	10.2087	3.0727	1.6378	0.8286	5.1968	4.2122	1.5552	0.3488	0.0356	0.0000	0.0388	0.0000
2C-15_89	13.3366	4.7687	3.8247	7.5314	11.3077	10.9214	9.3245	8.2960	4.8186	0.3694	0.1111	0.0407
3B-13_87	14.9069	4.7636	3.2676	3.6739	9.0353	8.8081	4.5146	5.0226	2.5122	0.0252	0.1632	0.0144
1A-9_89	28.1915	9.5589	0.1928	0.0565	17.8456	16.3882	0.0179	0.0000	0.0000	0.0000	0.1192	0.0845
1A-2_89	18.3109	6.0870	0.1291	0.0388	10.6207	9.5145	0.0120	0.0000	0.0000	0.0000	0.0778	0.0454
3C-6_89	8.9705	2.7010	1.3483	2.4168	3.8129	3.5986	2.7958	2.5017	1.5411	0.1030	0.0582	0.0082
3B-5_87	9.3743	2.7600	1.6932	1.7657	4.4234	4.1639	2.1737	2.3923	1.1130	0.0000	0.0715	0.0041
1B-6_89	24.0462	8.0619	0.1825	0.0698	14.4690	13.0997	0.0177	0.0000	0.0000	0.0000	0.1076	0.0736
3C-2_87	8.2958	2.4263	1.4986	1.5583	3.9046	3.6543	1.9451	2.1840	0.9933	0.0045	0.0682	0.0022
1A-15_89	32.8582	12.6442	0.3041	0.1512	30.6470	29.9818	0.0392	0.0000	0.0000	0.0000	0.2219	0.1834
3B-15_87	13.0034	4.6666	3.8532	4.7785	11.5288	11.8471	6.2052	7.2618	3.6735	0.0768	0.2485	0.0484
4A-5_87	10.4751	3.1553	1.7018	0.8355	5.3652	4.3455	1.5896	0.3540	0.0410	0.0000	0.0283	0.0000
1A-12_89	33.8588	11.7598	0.2449	0.0943	22.8166	21.1013	0.0205	0.0000	0.0000	0.0000	0.1429	0.1166
4C-8_87	11.9317	3.6193	1.9914	0.9724	6.1954	5.0734	1.8605	0.4616	0.0601	0.0000	0.0249	0.0000
2A-9_87	12.4332	3.7770	2.2535	2.4690	6.9554	6.6706	3.0976	3.6533	1.8560	0.0088	0.0673	0.0059

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
2B-13_89	14.2647	4.6264	3.0995	5.8520	9.0030	8.4276	7.0051	6.2393	3.8021	0.3169	0.0748	0.0225
2B-11_87	13.4728	4.1396	2.6124	2.8742	7.8902	7.6425	3.6641	4.3378	2.2456	0.0182	0.0724	0.0104
2B-8_89	9.0872	2.7367	1.5629	2.8042	4.3944	3.9555	3.2510	2.8037	1.6726	0.0714	0.0462	0.0068
4C-15_87	18.9023	6.4806	4.4332	2.4698	15.0884	13.2085	4.9539	1.5587	0.4971	0.0084	0.1085	0.0376
3C-10_89	11.1658	3.4023	1.7215	3.0540	4.9654	4.7444	3.6227	3.2974	2.1315	0.1483	0.0734	0.0116
3C-10_87	11.2019	3.3356	2.0534	2.1833	5.5416	5.2359	2.6635	2.9698	1.4213	0.0050	0.0884	0.0048
2A-5_89	8.0356	2.3987	1.3408	2.4058	3.7941	3.4079	2.8011	2.4258	1.4419	0.0800	0.0390	0.0066
4A-10_87	13.0073	3.9905	2.3139	1.1162	7.0248	5.7564	2.1765	0.6368	0.1518	0.0020	0.0328	0.0023
2C-8_89	7.6431	2.2895	1.2897	2.3468	3.6439	3.2708	2.7318	2.3923	1.4560	0.0535	0.0362	0.0023
3C-9_89	10.4131	3.1495	1.5737	2.8082	4.4988	4.2547	3.2779	2.8984	1.7761	0.1186	0.0640	0.0086
2B-9_87	12.6309	3.8623	2.3168	2.6077	7.3099	7.1141	3.3376	4.0603	2.0772	0.0136	0.0653	0.0000
3C-16_87	8.4963	3.5067	3.6807	5.1957	12.0209	13.5090	7.1532	9.0404	4.6347	0.1655	0.3263	0.0655
3A-1_89	7.3271	2.1859	1.0663	1.8610	2.9626	2.7587	2.1196	1.8224	0.9863	0.0147	0.0500	0.0019
3A-12_87	12.4899	3.7701	2.4028	2.6039	6.4045	6.0944	3.1521	3.5065	1.6345	0.0052	0.1037	0.0063
3B-15_87	12.8493	4.6085	3.8184	4.7571	11.4129	11.7292	6.2260	7.2229	3.6765	0.1131	0.2583	0.0501
2B-15_89	12.1181	4.5181	3.8830	8.1215	12.0979	12.0302	10.2278	9.5291	5.7698	0.4674	0.1322	0.0418
1B-11_89	32.3915	11.1901	0.2339	0.0999	21.2322	19.5520	0.0232	0.0000	0.0000	0.0000	0.1401	0.1126
2C-15_89	13.6853	4.9105	3.9942	8.0198	11.9823	11.6440	10.0002	9.2017	5.6286	0.4611	0.1189	0.0417
2A-6_87	11.0252	3.3588	1.8427	2.1747	6.2993	6.1641	2.7602	3.4520	1.7588	0.0000	0.0431	0.0000

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
4C-7_87	11.5213	3.4850	1.8853	0.9518	5.9506	4.8546	1.7507	0.4500	0.0642	0.0000	0.0229	0.0000
1B-5_87	21.0806	7.4604	0.1860	0.0678	13.6901	12.3871	0.0170	0.0000	0.0082	0.0000	0.0682	0.0491
2B-15_87	12.4090	4.7999	4.2432	5.6075	15.3927	16.6407	8.0310	10.7271	5.9566	0.2404	0.1619	0.0485
3C-17_89	7.8554	3.4748	3.7313	8.6315	11.9407	13.4531	11.8694	11.7922	7.1346	0.5233	0.2982	0.1072
4B-7_87	11.4584	3.4716	1.8756	0.9298	5.9925	4.9085	1.7886	0.4514	0.0549	0.0000	0.0204	0.0000
2B-9_89	8.9452	2.6900	1.5540	2.7902	4.3262	3.8865	3.2207	2.7628	1.6316	0.0773	0.0469	0.0080
1B-14_87	33.0373	12.9366	0.3842	0.2064	29.7861	28.6188	0.0431	0.0000	0.0000	0.0000	0.1715	0.1446
3B-18_89	0.1935	0.1928	1.2139	6.0645	5.6065	9.9027	13.7041	21.7308	16.0957	1.1604	0.6962	0.3157
3C-11_87	12.0321	3.6034	2.2886	2.4333	6.0759	5.7668	3.0048	3.3060	1.4960	0.0047	0.0976	0.0030
2B-14_87	15.9110	5.5494	3.9918	5.0932	14.8670	15.8183	7.2072	9.8317	5.6408	0.0309	0.1091	0.0102
2A-13_87	15.9216	5.0965	3.2827	3.8791	10.9129	10.9680	5.1731	6.5532	3.4705	0.0000	0.0660	0.0036
2A-14_87	16.7149	5.6317	3.8472	4.5939	13.2728	13.5031	6.1632	7.8983	4.2723	0.0332	0.1017	0.0186
2B-2_89	7.1678	2.1377	1.1312	2.1213	3.3868	3.0556	2.4978	2.2399	1.2643	0.0118	0.0144	0.0000
1B-18_87	9.4096	5.8019	0.2908	0.2416	33.5008	39.3234	0.0783	0.0151	0.0000	0.0000	0.4304	0.3965
3B-10_87	11.7042	3.4977	2.1308	2.2566	5.7644	5.4630	2.7347	2.9895	1.4264	0.0047	0.0894	0.0028
4C-7_87	11.5225	3.4845	1.8670	0.9218	5.9338	4.8539	1.7381	0.4482	0.0637	0.0000	0.0231	0.0000
1C-9_87	28.5670	10.2837	0.2321	0.0733	19.9960	18.5610	0.0227	0.0000	0.0000	0.0000	0.0769	0.0768
2B-12_89	11.1726	3.4601	2.0331	3.7641	6.0529	5.5482	4.4320	3.9132	2.4702	0.2187	0.0532	0.0152
1A-4_89	20.9083	7.0223	0.1413	0.0513	12.6027	11.4104	0.0155	0.0000	0.0000	0.0000	0.0847	0.0492

Sample	C8-monoaromatics A	C8-monoaromatics B	C9-alkanes A	C9-alkanes B	C9-monoaromatics A	C9-monoaromatics B	Heavy Alkanes A	Heavy Alkanes B	Heavy Alkanes C	Heavy Alkanes D	Heavy arom A	Heavy arom B
1B-18_87	9.6598	5.9850	0.2771	0.2433	35.2082	41.8335	0.0783	0.0000	0.0000	0.0000	0.4314	0.3971
1A-4_87	17.7944	6.1120	0.1847	0.0669	10.3277	9.1157	0.0154	0.0000	0.0000	0.0000	0.0739	0.0506
3B-1_89	7.3352	2.1855	1.0841	1.8716	2.9199	2.7215	2.1451	1.8290	1.0269	0.0181	0.0514	0.0018
1A-12_87	33.0459	12.0558	0.3124	0.1089	23.9118	22.1863	0.0375	0.0000	0.0000	0.0000	0.1169	0.0853
2B-11_87	13.9380	4.3024	2.6408	2.9597	8.3645	8.1860	3.8157	4.6310	2.3840	0.0053	0.0702	0.0079
3A-9_87	11.2236	3.3230	2.0670	2.1745	5.4419	5.1599	2.6652	2.9955	1.3786	0.0048	0.0867	0.0000
4A-10_87	13.3415	4.0797	2.2546	1.1352	7.1922	5.9303	2.1863	0.6144	0.1139	0.0000	0.0382	0.0023
4B-12_87	14.0312	4.3228	2.4216	1.2386	7.7635	6.4125	2.3547	0.6468	0.1226	0.0000	0.0320	0.0022
4A-13_87	17.3531	5.5324	3.3761	1.7885	10.8350	9.1838	3.4306	1.0615	0.2554	0.0000	0.0641	0.0090
3C-12_87	11.5984	3.4961	2.2716	2.4193	6.0030	5.7287	2.9547	3.2635	1.5225	0.0036	0.0784	0.0000
2C-17_89	1.5756	1.0180	2.6286	8.5030	9.8555	12.8237	14.0226	16.2891	10.4702	0.7581	0.3021	0.1303
3A-3_87	8.6917	2.5549	1.5848	1.6511	4.0718	3.7817	2.0375	2.2826	1.0183	0.0000	0.0659	0.0000
3C-17_89	8.0103	3.5573	3.7822	8.8108	12.3271	13.9264	12.0740	12.1680	7.4516	0.5497	0.3029	0.1140
2B-1_89	7.0960	2.1298	1.1337	2.1392	3.4569	3.1472	2.5254	2.3432	1.4448	0.0340	0.0281	0.0019
4A-8_87	11.5197	3.4937	1.9262	0.9776	6.0233	4.9495	1.8395	0.4543	0.0609	0.0000	0.0390	0.0019
1A-16_89	27.5023	11.6100	0.3104	0.1879	34.0897	35.7529	0.0471	0.0000	0.0000	0.0000	0.2809	0.2406

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2C-1_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2369	0.0059	0.1356	1
3C-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9848	0.0428	0.6934	1290
3C-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2529	0.0000	0.1831	60
2C-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.2143	0.0000	0.3270	480
3C-14_89	0.0117	0.0000	0.0038	0.0000	0.0000	0.0078	0.0000	0.9974	0.0430	0.4399	1680
1A-7_87	0.0223	0.0034	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2968	240
3B-13_89	0.0038	0.0000	0.0000	0.0000	0.0000	0.0067	0.0000	0.8467	0.0490	0.3628	1230
4C-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0400	0.0000	0.1982	1230
3A-15_89	0.0239	0.0000	0.0101	0.0010	0.0000	0.0111	0.0000	1.3743	0.1115	0.6106	2100
4B-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0072	0.0000	0.1015	180
2C-18_87	0.0482	0.0000	0.0244	0.0000	0.0000	0.0248	0.0126	8.8853	0.8098	1.9443	4320
4A-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0094	0.0000	0.0876	90
2C-18_87	0.0456	0.0000	0.0237	0.0000	0.0000	0.0255	0.0059	7.0715	0.6633	2.0325	4320
2A-19_87	0.0834	0.0029	0.0474	0.0074	0.0000	0.0411	0.0131	13.2913	1.4524	2.3343	4890
2A-16_87	0.0028	0.0000	0.0000	0.0000	0.0000	0.0075	0.0000	3.0855	0.2558	1.0760	2880
2B-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2670	0.0000	0.1465	60
4A-17_87	0.0657	0.0129	0.0087	0.0000	0.0000	0.0055	0.0018	0.3745	0.0051	0.6475	3540

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2B-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8140	0.0070	0.4177	480
3A-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4398	0.0054	0.3347	120
1A-7_89	0.0354	0.0091	0.0086	0.0000	0.0000	0.0000	0.0031	0.0040	0.0000	0.2881	240
1B-10_87	0.0285	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3456	495
2B-17_89	0.0546	0.0015	0.0324	0.0050	0.0000	0.0268	0.0142	3.0103	0.2745	1.3862	3560
3B-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5928	0.0101	0.4313	465
1A-12_87	0.0522	0.0097	0.0098	0.0000	0.0000	0.0075	0.0000	0.0000	0.0000	0.4227	720
1B-19_87	0.6220	0.3309	0.1493	0.1441	0.0129	0.0658	0.2574	0.3280	0.0187	1.8992	4980
3C-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6042	0.0080	0.4638	600
3A-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4690	0.0071	0.3530	180
1A-1_89	0.0109	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1828	1
1A-4_87	0.0167	0.0034	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2930	90
1A-15_87	0.1584	0.0551	0.0301	0.0094	0.0000	0.0189	0.0268	0.0303	0.0048	0.7876	2120
1C-4_87	0.0138	0.0026	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2426	90
3C-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5357	0.0052	0.3941	360
2B-2_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2576	0.0019	0.1379	30
1B-19_87	0.5574	0.3284	0.1516	0.1436	0.0385	0.0707	0.2565	0.2830	0.0237	1.9772	4980
2B-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0717	0.0082	0.3677	480
4A-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0729	0.0000	0.2611	1680

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3A-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4744	0.0084	0.3615	180
4C-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0044	0.0000	0.0793	60
4B-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0040	0.0000	0.0740	1
4C-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0050	0.0000	0.0904	120
3C-17_87	0.0170	0.0000	0.0075	0.0000	0.0000	0.0130	0.0000	2.8824	0.3068	1.8128	3540
3B-17_89	0.0780	0.0032	0.0380	0.0053	0.0000	0.0333	0.0141	3.4753	0.3874	1.2617	3540
1B-17_87	0.2610	0.0993	0.0487	0.0336	0.0000	0.0280	0.0737	0.0746	0.0066	1.0845	3530
2C-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2393	0.0050	0.1920	300
2C-13_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7674	0.0000	0.3474	1230
3C-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4231	0.0087	0.3261	60
2B-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5271	0.0000	0.2620	30
1A-11_89	0.0756	0.0101	0.0091	0.0000	0.0000	0.0000	0.0079	0.0000	0.0000	0.3665	600
3C-15_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.4691	0.1019	1.0450	2130
1B-1_87	0.0260	0.0031	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2348	1
1A-1_87	0.0092	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2145	1
2A-13_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7082	0.0087	0.4003	1230
3B-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3431	0.0024	0.2595	1
1B-17_89	0.4371	0.2316	0.0969	0.0794	0.0000	0.0504	0.2074	0.2244	0.0164	1.3092	3540
1A-6_89	0.0449	0.0059	0.0067	0.0000	0.0000	0.0049	0.0039	0.0031	0.0000	0.2880	180

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3B-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2163	0.0000	0.1799	60
1C-14_89	0.1290	0.0430	0.0231	0.0156	0.0000	0.0174	0.0215	0.0147	0.0000	0.5981	1680
3A-19_87	0.0482	0.0000	0.0245	0.0000	0.0000	0.0250	0.0000	4.5491	0.5428	2.5635	5010
3C-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2649	0.0022	0.1893	120
1C-8_89	0.0700	0.0063	0.0042	0.0000	0.0000	0.0056	0.0098	0.0033	0.0000	0.3402	300
3B-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6606	0.0184	0.5128	600
2A-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5491	0.0000	0.2500	90
3C-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4236	0.0035	0.2331	465
4C-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0057	0.0000	0.1241	600
1C-3_89	0.0247	0.0049	0.0047	0.0000	0.0000	0.0040	0.0000	0.0027	0.0000	0.2347	60
3B-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2463	0.0058	0.1804	120
2C-12_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5564	0.0063	0.2541	720
3B-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4670	0.0056	0.3600	180
3A-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2504	0.0000	0.1845	60
3B-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5736	0.0129	0.4424	360
3A-15_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.3752	0.0869	0.9669	2130
4A-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0093	0.0000	0.0984	180
1A-15_87	0.1510	0.0477	0.0283	0.0058	0.0000	0.0200	0.0402	0.0373	0.0045	0.7763	2120
2B-13_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8713	0.0061	0.4204	1230

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
1A-3_89	0.0344	0.0051	0.0055	0.0000	0.0000	0.0021	0.0000	0.0029	0.0000	0.2612	60
3C-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5517	0.0116	0.4177	465
2A-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.7833	0.0679	0.5218	1230
3C-2_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2092	0.0000	0.1440	30
4C-17_87	0.0610	0.0075	0.0050	0.0000	0.0000	0.0048	0.0000	0.3938	0.0041	0.6803	3540
2A-19_87	0.0855	0.0000	0.0487	0.0109	0.0000	0.0424	0.0303	12.1095	1.3020	2.3576	4890
1C-19_87	1.8705	1.0107	0.4431	0.5341	0.2387	0.2146	0.8329	1.0649	0.1242	3.7662	4980
4C-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0023	0.0000	0.1020	240
1C-4_87	0.0153	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2609	90
3A-14_89	0.0080	0.0000	0.0078	0.0000	0.0000	0.0091	0.0000	1.0917	0.0653	0.4781	1680
2C-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6858	0.0000	0.2676	90
4C-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0041	0.0000	0.0903	90
1C-8_87	0.0334	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2905	300
1B-12_89	0.0869	0.0201	0.0167	0.0070	0.0000	0.0080	0.0267	0.0063	0.0000	0.4535	720
3A-13_89	0.0026	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8384	0.0236	0.3973	1230
2B-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6006	0.0180	0.2798	60
3B-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3530	0.0030	0.2083	240
1B-16_87	0.1870	0.0615	0.0312	0.0103	0.0000	0.0227	0.0312	0.0482	0.0000	0.8214	2880
3A-16_89	0.0269	0.0000	0.0160	0.0000	0.0000	0.0157	0.0048	2.2646	0.1770	0.7823	2880

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3A-14_89	0.0096	0.0000	0.0052	0.0000	0.0000	0.0083	0.0000	1.2084	0.0650	0.4665	1680
3A-15_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.3451	0.0931	0.9670	2130
4B-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0126	0.0000	0.1341	720
1B-8_87	0.0274	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3041	300
3C-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4429	0.0060	0.3479	120
2C-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6782	0.0000	0.2597	90
3A-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2673	0.0024	0.1783	60
3A-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3190	0.0027	0.1966	180
2B-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6737	0.0000	0.2818	180
3A-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2822	0.0023	0.1894	120
3B-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3181	0.0060	0.2572	1
1B-12_87	0.0436	0.0074	0.0139	0.0000	0.0000	0.0093	0.0032	0.0038	0.0000	0.4519	720
1A-10_87	0.0368	0.0078	0.0000	0.0022	0.0000	0.0000	0.0000	0.0000	0.0000	0.3698	495
2C-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3383	0.0000	0.2053	1
2A-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7624	0.0205	0.3644	360
3B-16_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0084	0.0000	2.1576	0.2213	1.4681	2880
1C-15_89	0.1649	0.0669	0.0363	0.0103	0.0000	0.0212	0.0599	0.0370	0.0055	0.7222	2130
1B-3_89	0.0289	0.0042	0.0000	0.0000	0.0000	0.0037	0.0000	0.0026	0.0000	0.2344	60
2B-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3994	0.0000	0.1979	1

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3A-2_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2053	0.0000	0.1636	30
1C-17_87	0.3955	0.1890	0.0721	0.0626	0.0030	0.0433	0.1286	0.1031	0.0095	1.3753	3530
1A-16_89	0.2030	0.0913	0.0448	0.0301	0.0000	0.0247	0.0772	0.0439	0.0067	0.8198	2880
4B-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0042	0.0000	0.0846	30
1C-14_87	0.1361	0.0486	0.0237	0.0086	0.0000	0.0172	0.0280	0.0253	0.0000	0.7095	1680
1C-12_89	0.0966	0.0116	0.0174	0.0000	0.0000	0.0124	0.0283	0.0074	0.0000	0.4389	720
4C-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0147	0.0000	0.1285	720
2C-11_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4480	0.0078	0.2049	600
1B-9_89	0.0614	0.0070	0.0064	0.0000	0.0000	0.0065	0.0059	0.0049	0.0000	0.3588	360
2C-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2823	0.0020	0.1848	360
3B-15_89	0.0181	0.0000	0.0087	0.0000	0.0000	0.0090	0.0000	1.7030	0.1022	0.5879	2100
1B-3_87	0.0179	0.0034	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2704	60
4A-15_87	0.0092	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1406	0.0000	0.3197	2130
2A-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3225	0.0000	0.1731	180
1B-15_87	0.1429	0.0390	0.0256	0.0121	0.0000	0.0174	0.0267	0.0284	0.0000	0.6914	2120
1C-8_89	0.0490	0.0080	0.0064	0.0029	0.0000	0.0053	0.0063	0.0000	0.0000	0.3338	300
2C-19_87	0.0659	0.0000	0.0379	0.0059	0.0000	0.0291	0.0137	9.9208	1.0635	2.1950	4890
1A-15_89	0.1584	0.0473	0.0303	0.0090	0.0000	0.0187	0.0501	0.0266	0.0000	0.6381	2130
4A-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0120	0.0000	0.1068	300

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2C-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6497	0.0000	0.2706	90
3A-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4378	0.0074	0.3312	120
1A-13_87	0.0803	0.0278	0.0201	0.0024	0.0000	0.0138	0.0090	0.0150	0.0028	0.6147	1290
1A-3_89	0.0459	0.0053	0.0061	0.0000	0.0000	0.0038	0.0000	0.0030	0.0000	0.2752	60
4C-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0784	0.0000	0.2563	1680
4B-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0057	0.0000	0.1081	300
1C-1_87	0.0102	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2156	1
3B-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6970	0.0155	0.5115	600
3C-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0693	0.0888	0.7875	1680
3B-15_89	0.0198	0.0000	0.0047	0.0000	0.0000	0.0110	0.0000	1.6330	0.0815	0.5930	2100
2B-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.2539	0.0170	0.4456	720
2A-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.9315	0.0362	0.6770	1680
1B-16_89	0.3265	0.1354	0.0654	0.0485	0.0029	0.0346	0.1435	0.0888	0.0091	1.0752	2880
3C-15_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.4443	0.1103	1.0478	2130
1B-9_89	0.0686	0.0145	0.0096	0.0000	0.0000	0.0067	0.0043	0.0067	0.0000	0.3676	360
2B-18_89	0.1616	0.0133	0.0607	0.0199	0.0000	0.0529	0.0295	4.9538	0.4474	1.7313	4290
2A-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2935	0.0029	0.1631	120
2A-2_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2372	0.0000	0.1529	30
2B-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8366	0.0184	0.4146	480

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
1C-2_89	0.0297	0.0043	0.0000	0.0000	0.0000	0.0045	0.0000	0.0000	0.0000	0.2397	30
4A-17_87	0.0608	0.0065	0.0051	0.0000	0.0000	0.0000	0.0000	0.3669	0.0081	0.6494	3540
3A-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3511	0.0000	0.1906	300
1A-18_89	0.3914	0.1533	0.0950	0.0892	0.0029	0.0413	0.1571	0.2012	0.0111	1.2177	4320
3B-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4065	0.0000	0.2252	360
2B-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6500	0.0000	0.2621	120
3C-16_89	0.0270	0.0000	0.0108	0.0000	0.0000	0.0135	0.0000	1.5447	0.1312	0.7695	2880
1C-11_89	0.0761	0.0148	0.0123	0.0000	0.0000	0.0087	0.0195	0.0113	0.0000	0.4094	600
4B-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0066	0.0000	0.0859	60
3C-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5106	0.0053	0.3988	300
4B-14_87	0.0590	0.0021	0.0048	0.0000	0.0000	0.0000	0.0000	0.3276	0.0000	0.5944	1680
3C-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2367	0.0036	0.1979	120
3A-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6486	0.0088	0.4957	720
2A-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6302	0.0000	0.2516	120
3B-2_89	0.0000	0.0000	0.0000	0.0000	0.0011	0.0000	0.0000	0.2163	0.0054	0.1708	30
3A-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4077	0.0065	0.3124	90
3C-18_89	0.0713	0.0057	0.0347	0.0076	0.0000	0.0316	0.0121	3.3504	0.3697	1.2505	4290
3B-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5007	0.0083	0.3859	240
2B-17_89	0.0559	0.0000	0.0389	0.0066	0.0000	0.0301	0.0143	3.5085	0.2732	1.3273	3560

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2B-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5046	0.0000	0.2439	30
1A-19_89	0.6535	0.3340	0.1545	0.1644	0.0538	0.0723	0.2759	0.4510	0.0325	1.8136	5010
2C-18_89	0.1569	0.0192	0.0706	0.0191	0.0000	0.0608	0.0384	5.1427	0.4897	1.7806	4290
1B-18_89	3.9420	2.2200	1.0324	1.1868	0.7121	0.4572	2.0249	2.9522	0.7511	4.8595	4320
3B-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2472	0.0021	0.1899	90
3B-18_87	0.0738	0.0036	0.0330	0.0021	0.0000	0.0313	0.0000	5.2076	0.6968	2.7482	4320
2A-1_89	0.0000	0.0000	0.0000	0.0000	0.0113	0.0000	0.0000	0.2072	0.0000	0.1290	1
2B-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9427	0.0000	0.3163	300
2B-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2914	0.0030	0.2116	240
4A-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0072	0.0000	0.1047	240
3C-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3100	0.0000	0.1873	180
3A-18_89	0.1176	0.0061	0.0429	0.0111	0.0000	0.0376	0.0200	3.6318	0.3911	1.3339	4290
1B-16_87	0.1722	0.0624	0.0364	0.0139	0.0000	0.0221	0.0386	0.0397	0.0000	0.8293	2880
2C-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.5086	0.0322	0.5334	1230
3A-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4273	0.0039	0.2176	360
4B-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0064	0.0000	0.0908	120
2C-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2827	0.0021	0.1833	120
3B-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3206	0.0000	0.1705	180
2C-2_89	0.0000	0.0000	0.0000	0.0000	0.0071	0.0000	0.0019	0.1643	0.0000	0.1414	30

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2B-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3588	0.0025	0.2177	465
1A-1_87	0.0090	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2190	1
3A-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4999	0.0160	0.3774	240
1C-7_89	0.0529	0.0058	0.0056	0.0000	0.0000	0.0051	0.0000	0.0063	0.0000	0.3079	240
1A-8_89	0.0447	0.0033	0.0041	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3020	300
4C-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0028	0.0000	0.1067	300
3A-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5316	0.0029	0.4035	300
1C-11_89	0.0699	0.0140	0.0152	0.0000	0.0000	0.0072	0.0234	0.0106	0.0000	0.4268	600
2C-12_89	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5638	0.0093	0.2558	720
2B-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2555	0.0000	0.1686	60
3B-13_89	0.0059	0.0000	0.0036	0.0000	0.0000	0.0065	0.0000	0.8526	0.0483	0.3576	1230
1B-4_87	0.0191	0.0036	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2890	90
1B-15_87	0.1589	0.0461	0.0302	0.0128	0.0000	0.0177	0.0285	0.0345	0.0000	0.6918	2120
3A-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3241	0.0032	0.1936	240
1C-19_87	1.9249	1.0751	0.4482	0.5044	0.2562	0.2115	0.8307	1.0780	0.1547	3.7400	4980
1B-3_87	0.0129	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2554	60
2B-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5592	0.0169	0.2652	60
3A-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4691	0.0043	0.3629	180
2A-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7471	0.0000	0.3286	300

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
1B-9_89	0.0678	0.0059	0.0055	0.0000	0.0000	0.0069	0.0136	0.0042	0.0000	0.3602	360
1A-13_87	0.0863	0.0279	0.0129	0.0000	0.0000	0.0125	0.0077	0.0200	0.0031	0.6122	1290
3B-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4758	0.0054	0.3609	180
3C-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3869	0.0045	0.2976	30
2A-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2436	0.0018	0.1945	300
1A-8_89	0.0504	0.0063	0.0079	0.0000	0.0000	0.0061	0.0054	0.0042	0.0000	0.3123	300
2B-12_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5787	0.0031	0.2484	720
4C-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0094	0.0000	0.1223	720
3C-1_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1762	0.0000	0.1706	1
3C-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2204	0.0000	0.1949	60
2B-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3894	0.0000	0.1992	1
4B-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0022	0.0000	0.0874	60
2C-14_89	0.0026	0.0000	0.0000	0.0000	0.0000	0.0056	0.0000	0.8906	0.0173	0.4986	1680
1A-10_89	0.0665	0.0131	0.0114	0.0000	0.0000	0.0074	0.0116	0.0043	0.0000	0.3655	465
1C-3_87	0.0191	0.0019	0.0000	0.0000	0.0000	0.0018	0.0000	0.0015	0.0000	0.2699	60
2B-15_89	0.0030	0.0000	0.0000	0.0000	0.0000	0.0073	0.0000	1.3930	0.0477	0.6815	2100
3C-13_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0044	0.0000	0.7516	0.0253	0.4017	1230
1C-1_87	0.0101	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2137	1
2A-16_89	0.0207	0.0000	0.0030	0.0000	0.0000	0.0129	0.0000	1.9264	0.1034	0.8636	2880

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2B-11_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4508	0.0077	0.2476	600
1A-11_89	0.0773	0.0134	0.0134	0.0052	0.0000	0.0084	0.0216	0.0042	0.0000	0.4000	600
2A-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9399	0.0155	0.4108	600
1C-18_89	1.0621	0.5245	0.2707	0.2984	0.1102	0.1208	0.4995	0.7585	0.0504	2.4975	4320
1B-8_89	0.0639	0.0108	0.0085	0.0000	0.0000	0.0065	0.0071	0.0036	0.0000	0.3328	300
2A-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7383	0.0082	0.3197	240
1A-18_87	0.3812	0.1993	0.0965	0.0891	0.0063	0.0473	0.1282	0.1482	0.0117	2.0394	4320
1A-16_87	0.2484	0.0777	0.0421	0.0249	0.0000	0.0264	0.0902	0.0738	0.0075	0.9261	2880
1A-13_87	0.0881	0.0320	0.0184	0.0000	0.0000	0.0140	0.0163	0.0140	0.0000	0.5976	1290
4B-14_87	0.0532	0.0028	0.0000	0.0000	0.0000	0.0000	0.0000	0.3190	0.0000	0.5962	1680
2C-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0526	0.0374	0.3870	600
1A-14_87	0.1280	0.0318	0.0177	0.0087	0.0000	0.0158	0.0228	0.0246	0.0000	0.6668	1680
2B-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2668	0.0000	0.1675	120
3A-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5437	0.0068	0.4226	360
3B-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3696	0.0031	0.2144	300
2A-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3215	0.0024	0.1699	180
4A-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0133	0.0000	0.1091	300
1B-2_89	0.0323	0.0046	0.0036	0.0000	0.0000	0.0019	0.0000	0.0021	0.0000	0.2354	30
3B-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4308	0.0041	0.2291	465

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2A-16_89	0.0144	0.0000	0.0104	0.0000	0.0000	0.0125	0.0000	1.7734	0.0804	0.8858	2880
3B-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0342	0.0683	0.7329	1290
2C-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2018	0.0000	0.1415	60
4A-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0550	0.0000	0.1955	1230
3C-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5113	0.0044	0.3928	240
2C-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2935	0.0023	0.1796	360
3B-16_89	0.0310	0.0000	0.0226	0.0000	0.0000	0.0195	0.0094	2.4611	0.2033	0.8298	2880
3A-16_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.8231	0.1860	1.2731	2880
3C-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5157	0.0076	0.3849	240
3B-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3664	0.0028	0.2844	30
2C-16_87	0.0053	0.0000	0.0000	0.0000	0.0000	0.0083	0.0000	2.8460	0.1773	1.0500	2880
2A-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7784	0.0110	0.2822	180
1B-6_89	0.0496	0.0045	0.0085	0.0000	0.0000	0.0057	0.0096	0.0048	0.0000	0.3002	180
1C-10_87	0.0598	0.0071	0.0000	0.0000	0.0000	0.0064	0.0000	0.0000	0.0000	0.3743	495
3A-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5893	0.0134	0.4378	465
3B-1_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2344	0.0017	0.1675	1
2B-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3149	0.0043	0.1952	300
4C-16_87	0.0174	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2046	0.0000	0.4661	2880
1B-12_87	0.0630	0.0083	0.0081	0.0000	0.0000	0.0088	0.0061	0.0052	0.0000	0.4465	720

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2A-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2904	0.0000	0.1743	120
4A-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0189	0.0000	0.1302	600
2C-17_87	0.0172	0.0000	0.0086	0.0000	0.0000	0.0138	0.0000	4.6638	0.4370	1.3821	3540
3B-15_89	0.0140	0.0000	0.0109	0.0000	0.0000	0.0109	0.0000	1.5229	0.1320	0.6185	2100
3C-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2620	0.0000	0.1835	120
4C-18_87	0.1437	0.0304	0.0157	0.0041	0.0000	0.0120	0.0030	0.6547	0.0401	1.1170	4320
2B-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0013	0.0000	0.2910	0.0021	0.2250	360
1B-1_87	0.0110	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2394	1
2A-1_89	0.0000	0.0000	0.0000	0.0000	0.0048	0.0000	0.0000	0.2206	0.0000	0.1379	1
3B-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4934	0.0106	0.3878	240
2A-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2583	0.0000	0.1723	90
3A-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0612	0.0737	0.7564	1680
2C-1_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2286	0.0055	0.1408	1
3B-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5538	0.0032	0.4158	300
3C-16_87	0.0092	0.0000	0.0000	0.0000	0.0000	0.0074	0.0000	2.0081	0.2162	1.4027	2880
2A-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6714	0.0000	0.2575	120
4A-18_87	0.2543	0.0806	0.0397	0.0187	0.0000	0.0223	0.0254	0.9817	0.0855	1.4583	4320
3C-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4940	0.0065	0.3956	300
2C-2_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2363	0.0000	0.1508	30

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3B-14_89	0.0113	0.0000	0.0088	0.0000	0.0000	0.0097	0.0000	1.0918	0.0733	0.4861	1680
1C-16_87	0.2316	0.0719	0.0415	0.0232	0.0000	0.0282	0.0607	0.0344	0.0077	0.9963	2880
1A-9_87	0.0402	0.0062	0.0030	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3366	360
3B-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4271	0.0036	0.2216	360
4C-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0063	0.0000	0.0920	180
1C-3_87	0.0121	0.0017	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2634	60
2C-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4358	0.0000	0.2367	30
2C-17_89	0.0623	0.0000	0.0317	0.0052	0.0000	0.0261	0.0135	2.9495	0.2307	1.2470	3560
2B-16_89	0.0341	0.0000	0.0148	0.0000	0.0000	0.0154	0.0037	1.7922	0.1351	1.1002	2880
1B-11_87	0.0515	0.0085	0.0079	0.0000	0.0000	0.0062	0.0030	0.0045	0.0000	0.4116	600
1C-5_89	0.0412	0.0052	0.0050	0.0000	0.0000	0.0056	0.0000	0.0000	0.0000	0.2570	120
1C-9_89	0.0430	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3083	360
3C-15_89	0.0107	0.0000	0.0023	0.0000	0.0000	0.0080	0.0000	1.3393	0.0675	0.5312	2100
4B-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0164	0.0000	0.1237	480
4A-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0045	0.0000	0.0839	60
2B-18_89	0.1578	0.0127	0.0613	0.0209	0.0000	0.0540	0.0261	5.1084	0.4731	1.6974	4290
3A-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0730	0.0637	0.7568	1680
2C-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7901	0.0041	0.3767	360
3B-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3732	0.0038	0.2064	300

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2C-2_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2547	0.0000	0.1385	30
3C-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5032	0.0071	0.3848	240
1B-19_87	0.6579	0.3298	0.1329	0.1459	0.0094	0.0716	0.2433	0.2744	0.0233	1.8133	4980
1B-7_89	0.0447	0.0053	0.0031	0.0000	0.0000	0.0054	0.0000	0.0000	0.0000	0.2944	240
2B-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2939	0.0021	0.1636	120
3C-19_89	0.1521	0.0246	0.0617	0.0205	0.0000	0.0535	0.0274	5.1344	0.5912	1.7520	4830
4C-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0066	0.0000	0.1154	600
3C-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3144	0.0000	0.2496	1
2C-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7652	0.0161	0.3762	360
2A-17_87	0.0172	0.0000	0.0136	0.0000	0.0000	0.0138	0.0000	4.3318	0.3702	1.3785	3540
4C-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0053	0.0000	0.1174	360
4B-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0069	0.0000	0.0922	120
3C-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3311	0.0029	0.1738	240
2B-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3150	0.0000	0.1701	180
3C-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5168	0.0061	0.3960	360
4B-14_87	0.0465	0.0021	0.0000	0.0000	0.0000	0.0000	0.0000	0.3142	0.0000	0.6407	1680
1A-2_89	0.0137	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2210	30
2C-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2732	0.0000	0.1640	120
1A-13_89	0.1084	0.0186	0.0198	0.0000	0.0000	0.0106	0.0141	0.0083	0.0000	0.5054	1290

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
1B-5_87	0.0277	0.0061	0.0024	0.0000	0.0000	0.0039	0.0000	0.0000	0.0000	0.2560	120
4B-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0066	0.0000	0.1394	720
4A-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0086	0.0000	0.0977	180
2B-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6324	0.0000	0.2455	120
1C-7_87	0.0244	0.0053	0.0000	0.0000	0.0000	0.0028	0.0000	0.0000	0.0000	0.3170	240
2B-13_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7344	0.0031	0.4479	1230
3C-13_89	0.0051	0.0000	0.0000	0.0000	0.0000	0.0059	0.0000	0.8337	0.0362	0.3555	1230
3A-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3942	0.0068	0.3034	30
1B-7_87	0.0269	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2743	240
3C-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4856	0.0093	0.3603	180
3C-19_89	0.1604	0.0243	0.0642	0.0214	0.0000	0.0559	0.0292	5.4610	0.6252	1.7157	4830
3A-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5517	0.0272	0.4010	300
3A-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3173	0.0031	0.1972	300
1B-5_89	0.0427	0.0049	0.0051	0.0000	0.0000	0.0045	0.0000	0.0036	0.0000	0.2726	120
2A-13_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7464	0.0053	0.3982	1230
1B-10_89	0.0670	0.0105	0.0044	0.0000	0.0000	0.0071	0.0088	0.0055	0.0000	0.3910	465
3A-16_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0034	0.0000	1.8375	0.1806	1.2708	2880
3C-2_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2148	0.0000	0.1636	30
2A-14_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.3598	0.0111	0.5013	1680

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2A-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5134	0.0000	0.2622	90
2B-19_87	0.1420	0.0068	0.0680	0.0252	0.0000	0.0564	0.0438	15.2344	1.7137	2.5811	4890
3B-11_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5236	0.0084	0.2613	600
3A-18_89	0.1078	0.0045	0.0393	0.0089	0.0000	0.0338	0.0149	3.6432	0.3750	1.3513	4290
4C-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0039	0.0000	0.0789	30
4C-17_87	0.0540	0.0021	0.0045	0.0000	0.0000	0.0051	0.0000	0.3820	0.0019	0.6810	3540
1C-3_89	0.0348	0.0052	0.0057	0.0000	0.0000	0.0020	0.0032	0.0000	0.0000	0.2390	60
4C-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0047	0.0000	0.0976	180
4B-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0068	0.0000	0.1055	300
3B-16_89	0.0463	0.0000	0.0199	0.0000	0.0000	0.0175	0.0092	2.2912	0.2168	0.8649	2880
2C-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7021	0.0000	0.3078	240
3C-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0977	0.0616	0.7883	1680
1C-17_89	0.4805	0.1838	0.1052	0.1084	0.0048	0.0507	0.2124	0.2237	0.0181	1.2733	3540
4A-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0049	0.0000	0.0967	120
3C-18_87	0.0485	0.0000	0.0185	0.0000	0.0000	0.0229	0.0000	4.1586	0.5177	2.4341	4320
4A-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0100	0.0000	0.1388	720
1B-15_87	0.1302	0.0280	0.0179	0.0000	0.0000	0.0150	0.0085	0.0083	0.0000	0.6542	2120
3B-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5720	0.0034	0.4292	360
4C-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0060	0.0000	0.1035	300

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
4B-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0043	0.0000	0.0705	1
3A-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4839	0.0043	0.2386	465
1B-7_87	0.0240	0.0058	0.0000	0.0000	0.0000	0.0044	0.0000	0.0000	0.0000	0.3119	240
2B-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3048	0.0022	0.2257	300
3B-17_87	0.0226	0.0000	0.0087	0.0000	0.0000	0.0161	0.0000	3.3301	0.3742	2.0509	3540
2C-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2365	0.0000	0.1679	90
2B-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3191	0.0021	0.1698	180
3B-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4626	0.0159	0.3530	180
1A-5_89	0.0366	0.0050	0.0028	0.0000	0.0000	0.0000	0.0000	0.0033	0.0000	0.2520	120
4B-16_87	0.1356	0.0397	0.0156	0.0067	0.0000	0.0135	0.0029	0.6454	0.0462	1.0257	2880
2B-17_87	0.0163	0.0000	0.0160	0.0000	0.0000	0.0169	0.0000	6.4599	0.5845	1.5473	3540
4B-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0053	0.0000	0.1041	360
2B-15_89	0.0073	0.0000	0.0000	0.0000	0.0000	0.0095	0.0000	1.4064	0.0328	0.6828	2100
4A-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0042	0.0000	0.0793	30
1A-14_87	0.1043	0.0266	0.0206	0.0092	0.0000	0.0155	0.0144	0.0237	0.0034	0.6713	1680
2B-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.5015	0.0314	0.6081	1230
3B-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6733	0.0141	0.5006	600
1C-10_89	0.0604	0.0123	0.0079	0.0000	0.0000	0.0074	0.0000	0.0052	0.0000	0.3565	465
2B-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8673	0.0000	0.2936	240

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2B-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6204	0.0000	0.2796	90
1C-7_87	0.0198	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2882	240
1C-4_89	0.0255	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2188	90
3A-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5811	0.0053	0.4283	465
4A-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0731	0.0000	0.2515	1680
2C-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3719	0.0028	0.2279	465
1A-3_87	0.0137	0.0000	0.0000	0.0000	0.0000	0.0018	0.0000	0.0000	0.0000	0.2726	60
3C-19_87	0.1155	0.0021	0.0462	0.0067	0.0000	0.0437	0.0171	6.7370	0.9019	3.0442	5010
3B-18_89	0.1479	0.0190	0.0601	0.0175	0.0000	0.0529	0.0277	4.9014	0.5307	1.7052	4290
4C-15_87	0.0058	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1273	0.0000	0.3209	2130
1B-7_89	0.0438	0.0079	0.0038	0.0000	0.0000	0.0055	0.0000	0.0000	0.0000	0.2895	240
3A-18_87	0.0280	0.0000	0.0122	0.0000	0.0000	0.0183	0.0000	3.6646	0.4409	2.1623	4320
4A-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0719	1
1B-11_89	0.0737	0.0206	0.0063	0.0000	0.0000	0.0113	0.0212	0.0087	0.0000	0.4275	600
1B-2_89	0.0233	0.0021	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2193	30
3A-17_87	0.0108	0.0000	0.0000	0.0000	0.0000	0.0082	0.0000	2.1541	0.2343	1.4536	3540
2C-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6231	0.0000	0.3083	180
3C-1_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2226	0.0000	0.1619	1
4C-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0681	1

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
1C-11_89	0.0735	0.0100	0.0115	0.0000	0.0000	0.0094	0.0202	0.0105	0.0000	0.4188	600
1B-11_87	0.0633	0.0088	0.0062	0.0000	0.0000	0.0079	0.0023	0.0035	0.0000	0.4317	600
2A-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6771	0.0137	0.3297	240
2B-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7329	0.0000	0.2842	180
1A-9_87	0.0191	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3106	360
1C-13_89	0.1392	0.0617	0.0275	0.0150	0.0000	0.0150	0.0396	0.0524	0.0030	0.6074	1290
2A-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8837	0.0000	0.3716	480
1C-18_87	0.7504	0.4251	0.1835	0.1939	0.0503	0.0860	0.3158	0.4244	0.0201	2.2459	4320
1A-16_87	0.2092	0.0731	0.0451	0.0260	0.0000	0.0251	0.0713	0.0673	0.0072	0.9334	2880
2C-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2935	0.0000	0.1559	180
1C-13_87	0.1098	0.0266	0.0225	0.0100	0.0000	0.0147	0.0155	0.0174	0.0000	0.5999	1290
1A-12_89	0.0854	0.0245	0.0155	0.0044	0.0000	0.0124	0.0154	0.0135	0.0000	0.4323	720
3A-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6281	0.0136	0.4807	600
4B-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0447	0.0000	0.1823	1230
1A-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2523	180
3B-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4329	0.0051	0.2359	465
2B-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5077	0.0000	0.2702	90
2C-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.3100	0.0344	0.5489	1230
2A-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.3682	0.0191	0.4053	720

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3A-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9349	0.0311	0.6809	1290
2B-17_89	0.0573	0.0016	0.0246	0.0037	0.0000	0.0280	0.0109	2.6932	0.2219	1.4368	3560
1A-17_89	0.2664	0.1189	0.0646	0.0408	0.0000	0.0308	0.1080	0.1207	0.0084	0.9618	3540
2B-19_87	0.1441	0.0193	0.0643	0.0205	0.0000	0.0552	0.0400	13.3959	1.5740	2.6086	4890
2C-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4150	0.0033	0.2238	465
1B-11_87	0.0584	0.0093	0.0120	0.0000	0.0000	0.0073	0.0038	0.0055	0.0000	0.4492	600
2A-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3049	0.0084	0.1489	90
2B-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3640	0.0022	0.2223	465
1A-9_89	0.0638	0.0081	0.0121	0.0000	0.0000	0.0061	0.0200	0.0038	0.0000	0.3541	360
2C-11_87	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8484	0.0273	0.4314	600
1A-14_87	0.1268	0.0321	0.0184	0.0083	0.0000	0.0152	0.0081	0.0269	0.0030	0.6964	1680
4C-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0083	0.0000	0.0976	180
2A-12_89	0.0012	0.0000	0.0000	0.0000	0.0000	0.0017	0.0000	0.5275	0.0092	0.2643	720
4C-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0068	0.0000	0.0900	120
3C-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4747	0.0075	0.3667	180
2C-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3661	0.0000	0.2085	1
3A-19_89	0.1819	0.0254	0.0698	0.0266	0.0000	0.0615	0.0313	5.9541	0.6941	1.6021	4830
1A-19_89	0.6158	0.3603	0.1623	0.1636	0.0407	0.0735	0.2949	0.4073	0.0249	1.7678	5010
2C-15_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	2.6439	0.0731	0.7783	2130

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3C-16_87	0.0078	0.0000	0.0000	0.0000	0.0000	0.0059	0.0000	2.0194	0.2122	1.4000	2880
1C-11_87	0.0455	0.0080	0.0071	0.0000	0.0000	0.0065	0.0000	0.0000	0.0000	0.4091	600
3A-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4157	0.0000	0.1954	360
2C-15_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0049	0.0000	2.3284	0.1218	0.8542	2130
2A-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3294	0.0000	0.1821	240
4A-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0069	0.0000	0.0785	60
3B-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3961	0.0030	0.2088	360
1C-8_89	0.0691	0.0109	0.0058	0.0052	0.0000	0.0068	0.0194	0.0069	0.0000	0.3407	300
2A-18_87	0.0292	0.0000	0.0218	0.0000	0.0000	0.0239	0.0072	8.2376	0.8193	1.8752	4320
2A-18_87	0.0433	0.0000	0.0257	0.0000	0.0000	0.0244	0.0118	7.1851	0.7111	1.9380	4320
1C-11_87	0.0665	0.0095	0.0082	0.0000	0.0000	0.0084	0.0057	0.0049	0.0000	0.4148	600
4A-16_87	0.0350	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2290	0.0000	0.4518	2880
1A-11_87	0.0426	0.0082	0.0040	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4021	600
2B-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.5207	0.0095	0.4416	720
3A-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2593	0.0000	0.1800	60
2A-14_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.1864	0.0000	0.5162	1680
1C-1_89	0.0199	0.0020	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1996	1
1C-2_87	0.0121	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2336	30
2A-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3196	0.0022	0.1940	360

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3A-16_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0070	0.0000	1.8176	0.1879	1.2730	2880
1A-17_87	0.3182	0.1239	0.0568	0.0349	0.0000	0.0355	0.1029	0.1226	0.0068	1.2652	3530
1C-2_87	0.0101	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2363	30
2C-17_87	0.0104	0.0000	0.0105	0.0000	0.0000	0.0148	0.0000	5.2139	0.4771	1.3537	3540
2B-14_89	0.0027	0.0000	0.0000	0.0000	0.0000	0.0028	0.0000	1.0439	0.0375	0.5684	1680
3C-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3144	0.0022	0.2514	1
3B-16_89	0.0478	0.0000	0.0182	0.0000	0.0000	0.0189	0.0092	2.2963	0.2224	0.8562	2880
3C-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4635	0.0061	0.3368	120
3B-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3145	0.0000	0.1910	180
4A-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0060	0.0000	0.0839	30
3A-13_89	0.0028	0.0000	0.0000	0.0000	0.0000	0.0052	0.0000	0.9384	0.0314	0.4009	1230
3C-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2259	0.0019	0.1889	60
4B-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0055	0.0000	0.1066	300
1A-18_87	0.3743	0.2249	0.0909	0.0721	0.0102	0.0473	0.1245	0.1680	0.0105	2.0309	4320
1A-10_87	0.0379	0.0080	0.0000	0.0000	0.0000	0.0058	0.0000	0.0000	0.0000	0.3570	495
2B-1_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2445	0.0000	0.1347	1
1C-17_87	0.4059	0.1739	0.0833	0.0657	0.0033	0.0433	0.1350	0.1155	0.0104	1.3788	3530
1C-12_89	0.0869	0.0216	0.0173	0.0053	0.0000	0.0094	0.0129	0.0093	0.0000	0.4451	720
2C-19_87	0.0596	0.0041	0.0362	0.0046	0.0000	0.0322	0.0087	8.5642	0.8768	2.2616	4890

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2B-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6687	0.0081	0.2735	120
1B-17_87	0.2733	0.0897	0.0463	0.0270	0.0000	0.0279	0.0776	0.0857	0.0000	1.0729	3530
2A-10_89	0.0000	0.0000	0.0000	0.0000	0.0018	0.0000	0.0000	0.3483	0.0026	0.2100	465
1C-3_89	0.0184	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2283	60
3C-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3649	0.0063	0.1950	240
1B-8_87	0.0141	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2948	300
1A-3_89	0.0438	0.0047	0.0064	0.0000	0.0000	0.0043	0.0000	0.0028	0.0000	0.2583	60
1A-10_87	0.0246	0.0041	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3541	495
1B-2_87	0.0087	0.0016	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2454	30
2B-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	2.4471	0.0768	0.7121	1680
3A-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5161	0.0068	0.3769	240
3A-17_89	0.0617	0.0000	0.0217	0.0000	0.0000	0.0202	0.0045	2.4885	0.2330	1.0823	3540
3A-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4427	0.0038	0.2447	465
2C-1_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2381	0.0000	0.1415	1
1B-13_87	0.0806	0.0182	0.0113	0.0000	0.0000	0.0129	0.0084	0.0123	0.0027	0.6195	1290
3A-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3193	0.0033	0.2466	1
1C-11_87	0.0626	0.0071	0.0036	0.0000	0.0000	0.0059	0.0076	0.0040	0.0000	0.4245	600
3A-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4064	0.0077	0.3145	60
2C-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3341	0.0000	0.2083	1

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2C-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6327	0.0000	0.2643	60
1C-18_89	1.0484	0.5837	0.2542	0.2779	0.1294	0.1134	0.4687	0.6657	0.0542	2.5426	4320
4A-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0112	0.0000	0.1159	360
4C-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0040	0.0000	0.0768	60
2A-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7824	0.0206	0.4393	600
3C-15_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.4881	0.1073	1.0467	2130
2A-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7009	0.0107	0.3458	300
4A-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0590	0.0000	0.2084	1230
3B-12_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5669	0.0140	0.2522	720
1C-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2733	240
3C-18_87	0.0462	0.0000	0.0230	0.0000	0.0000	0.0211	0.0000	4.1476	0.5306	2.4288	4320
3C-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4428	0.0075	0.3454	120
2A-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5236	0.0000	0.2551	60
1C-4_89	0.0294	0.0043	0.0053	0.0000	0.0000	0.0042	0.0042	0.0000	0.0000	0.2439	90
2B-2_87	0.0017	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5165	0.0147	0.2565	30
2A-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8064	0.0091	0.3103	240
3B-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4531	0.0072	0.3391	120
3C-17_87	0.0161	0.0000	0.0050	0.0000	0.0000	0.0132	0.0000	2.9054	0.3137	1.8178	3540
3C-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4177	0.0031	0.3217	90

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3B-14_89	0.0125	0.0000	0.0040	0.0000	0.0000	0.0083	0.0000	1.1634	0.0605	0.4745	1680
2B-15_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	3.3671	0.0993	0.9304	2130
1B-6_87	0.0171	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2676	180
3B-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.2796	0.0809	0.9088	1680
2A-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6720	0.0000	0.2415	120
4A-15_87	0.0020	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1251	0.0000	0.3473	2130
2A-18_87	0.0267	0.0000	0.0241	0.0000	0.0000	0.0252	0.0000	8.0102	0.8021	1.8293	4320
1B-16_89	0.3215	0.1276	0.0621	0.0397	0.0000	0.0383	0.1107	0.0904	0.0147	0.9888	2880
2C-11_89	0.0000	0.0000	0.0000	0.0000	0.0012	0.0000	0.0000	0.4705	0.0056	0.2215	600
4A-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0096	0.0000	0.1113	360
2A-11_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5266	0.0099	0.2424	600
1C-10_87	0.0342	0.0076	0.0042	0.0000	0.0000	0.0065	0.0000	0.0000	0.0000	0.3763	495
4B-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0376	0.0000	0.2012	1230
3A-19_89	0.1896	0.0261	0.0718	0.0272	0.0000	0.0611	0.0332	6.0381	0.6783	1.6109	4830
4C-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0372	0.0000	0.1710	1230
4A-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0188	0.0000	0.1393	720
2A-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3560	0.0000	0.2305	465
2B-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9090	0.0000	0.3109	300
2B-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2981	0.0000	0.1780	180

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
1B-15_89	0.1820	0.0670	0.0413	0.0146	0.0000	0.0206	0.0680	0.0286	0.0108	0.7163	2130
1B-5_87	0.0249	0.0047	0.0000	0.0000	0.0000	0.0040	0.0000	0.0000	0.0000	0.2659	120
4C-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0042	0.0000	0.0920	120
2C-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.3100	0.0244	0.4446	720
2C-16_89	0.0259	0.0000	0.0142	0.0000	0.0000	0.0144	0.0036	1.8072	0.1359	0.9103	2880
2A-17_87	0.0199	0.0000	0.0114	0.0000	0.0000	0.0149	0.0000	4.5235	0.4012	1.3886	3540
2A-16_87	0.0028	0.0000	0.0000	0.0000	0.0000	0.0080	0.0000	3.7071	0.2411	1.0436	2880
2A-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5345	0.0000	0.2515	60
3A-12_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5395	0.0103	0.2984	720
1A-10_89	0.0518	0.0064	0.0077	0.0000	0.0000	0.0057	0.0055	0.0049	0.0000	0.3631	465
3C-12_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5022	0.0074	0.2579	720
2A-15_89	0.0052	0.0000	0.0000	0.0000	0.0000	0.0064	0.0000	1.2223	0.0340	0.6662	2100
1B-14_87	0.1236	0.0348	0.0158	0.0096	0.0000	0.0150	0.0173	0.0248	0.0000	0.6910	1680
3B-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2904	0.0052	0.1895	180
1B-1_87	0.0206	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2360	1
2B-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6115	0.0000	0.2711	90
4C-15_87	0.0042	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0971	0.0000	0.3181	2130
2C-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6489	0.0000	0.3203	240
1A-8_89	0.0395	0.0035	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2879	300

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2C-11_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4315	0.0072	0.2263	600
2C-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5714	0.0143	0.3395	300
1A-19_87	1.1646	0.6243	0.2669	0.2842	0.1110	0.1219	0.4431	0.5756	0.0641	3.0817	4980
1A-16_87	0.2442	0.0742	0.0418	0.0267	0.0000	0.0245	0.0770	0.0717	0.0051	0.9850	2880
3C-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9514	0.0332	0.6953	1290
3C-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3702	0.0027	0.2041	300
3B-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9966	0.0851	0.7316	1290
4A-18_87	0.2702	0.0854	0.0454	0.0234	0.0000	0.0214	0.0301	1.0037	0.0975	1.4566	4320
2C-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	2.0639	0.0297	0.6389	1680
3A-18_87	0.0385	0.0000	0.0174	0.0000	0.0000	0.0178	0.0000	3.5022	0.4255	2.1226	4320
2B-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.1697	0.0267	0.4677	720
1C-17_87	0.3662	0.1487	0.0794	0.0540	0.0066	0.0426	0.1088	0.1511	0.0075	1.4825	3530
2C-18_89	0.1579	0.0238	0.0690	0.0200	0.0000	0.0575	0.0375	4.8395	0.5009	1.7945	4290
3B-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4086	0.0029	0.3149	60
2B-16_87	0.0136	0.0000	0.0050	0.0000	0.0000	0.0130	0.0000	3.7418	0.3168	1.3150	2880
3A-14_89	0.0104	0.0000	0.0039	0.0000	0.0000	0.0082	0.0000	1.1947	0.0549	0.4699	1680
3A-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0579	0.0695	0.7531	1680
2C-16_87	0.0066	0.0000	0.0000	0.0000	0.0000	0.0077	0.0000	2.9296	0.1840	1.0717	2880
3B-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3765	0.0036	0.2012	240

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3B-2_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2367	0.0000	0.1665	30
2A-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9655	0.0177	0.4131	600
1A-15_89	0.1441	0.0587	0.0330	0.0129	0.0000	0.0182	0.0497	0.0445	0.0053	0.6565	2130
3A-17_89	0.0488	0.0000	0.0193	0.0000	0.0000	0.0189	0.0085	2.0126	0.1844	1.1420	3540
3C-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4844	0.0067	0.3602	180
1C-6_89	0.0131	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2505	180
3A-11_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5026	0.0000	0.2466	600
2A-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3152	0.0000	0.1927	360
2A-11_89	0.0012	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5295	0.0107	0.2630	600
4B-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0082	0.0000	0.1142	360
1A-18_89	0.3803	0.1733	0.0912	0.0829	0.0039	0.0408	0.1625	0.2329	0.0114	1.2156	4320
4A-17_87	0.0596	0.0000	0.0044	0.0000	0.0000	0.0039	0.0000	0.3625	0.0043	0.6490	3540
2A-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2502	0.0000	0.1236	60
3C-14_89	0.0026	0.0000	0.0044	0.0000	0.0000	0.0032	0.0000	1.0437	0.0237	0.4330	1680
2B-18_87	0.0615	0.0000	0.0371	0.0000	0.0000	0.0284	0.0139	9.7582	0.9426	2.1163	4320
1B-13_87	0.1026	0.0205	0.0125	0.0045	0.0000	0.0131	0.0180	0.0182	0.0029	0.5949	1290
2A-18_89	0.1094	0.0084	0.0436	0.0098	0.0000	0.0383	0.0182	4.1025	0.3514	1.5661	4290
4C-17_87	0.0618	0.0068	0.0044	0.0000	0.0000	0.0037	0.0000	0.3808	0.0022	0.6832	3540
2B-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3028	0.0000	0.1615	120

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2A-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3203	0.0022	0.1988	360
4B-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0053	0.0000	0.1021	240
3B-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2504	0.0000	0.1739	90
2C-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3029	0.0000	0.1605	180
2C-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2568	0.0000	0.1803	300
3C-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4789	0.0038	0.2231	465
3A-1_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1993	0.0000	0.1643	1
1B-14_87	0.0995	0.0213	0.0155	0.0000	0.0000	0.0139	0.0079	0.0073	0.0000	0.6278	1680
2B-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3521	0.0000	0.2184	1
3C-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2528	0.0000	0.1699	90
4B-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0149	0.0000	0.1183	480
2B-12_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5334	0.0088	0.2564	720
1B-10_89	0.0703	0.0144	0.0120	0.0000	0.0000	0.0072	0.0176	0.0051	0.0000	0.3866	465
3A-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4474	0.0062	0.2440	465
1C-8_87	0.0357	0.0061	0.0028	0.0000	0.0000	0.0054	0.0000	0.0000	0.0000	0.3168	300
3C-19_87	0.1209	0.0042	0.0449	0.0132	0.0000	0.0454	0.0205	6.6627	0.9083	3.0409	5010
1C-6_87	0.0172	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2771	180
2A-8_89	0.0000	0.0012	0.0000	0.0000	0.0000	0.0000	0.0000	0.2725	0.0079	0.2023	300
3C-12_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4930	0.0035	0.2605	720

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3C-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3116	0.0028	0.1903	180
3A-17_89	0.0618	0.0000	0.0186	0.0000	0.0000	0.0201	0.0085	2.3516	0.2222	1.0856	3540
1B-1_89	0.0214	0.0022	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1995	1
3A-19_89	0.1393	0.0241	0.0631	0.0190	0.0000	0.0528	0.0253	4.9520	0.5740	1.7878	4830
1B-2_87	0.0121	0.0016	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2443	30
2C-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.3663	0.0000	0.4282	720
3B-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2411	0.0021	0.1830	120
3C-18_89	0.0869	0.0014	0.0319	0.0049	0.0000	0.0290	0.0114	2.9928	0.3150	1.2906	4290
3B-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3766	0.0066	0.2863	30
3B-11_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5124	0.0080	0.2588	600
3A-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4036	0.0041	0.2140	360
1B-6_89	0.0515	0.0080	0.0093	0.0000	0.0000	0.0056	0.0099	0.0034	0.0000	0.3011	180
3A-11_89	0.0000	0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.4563	0.0069	0.2468	600
4C-18_87	0.1284	0.0307	0.0139	0.0045	0.0000	0.0121	0.0028	0.6742	0.0432	1.1156	4320
3C-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2520	0.0000	0.1686	90
1A-7_87	0.0317	0.0069	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3019	240
4A-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0754	0.0000	0.2594	1680
3C-16_89	0.0260	0.0000	0.0111	0.0000	0.0000	0.0135	0.0000	1.6519	0.1429	0.7448	2880
4A-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0220	0.0000	0.1296	480

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
1C-2_87	0.0109	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0029	0.0000	0.2348	30
1C-9_89	0.0596	0.0069	0.0061	0.0000	0.0000	0.0060	0.0059	0.0000	0.0000	0.3447	360
2B-17_87	0.0249	0.0000	0.0136	0.0000	0.0000	0.0170	0.0048	6.0414	0.5441	1.5602	3540
1B-2_87	0.0113	0.0018	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2389	30
1A-15_87	0.1498	0.0366	0.0334	0.0063	0.0000	0.0187	0.0337	0.0320	0.0046	0.7701	2120
1A-6_89	0.0504	0.0053	0.0059	0.0000	0.0000	0.0045	0.0000	0.0028	0.0000	0.2893	180
4C-16_87	0.0251	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2244	0.0000	0.4340	2880
3C-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6085	0.0083	0.4639	600
4C-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0017	0.0000	0.0666	1
1C-16_89	0.2767	0.1096	0.0550	0.0362	0.0000	0.0300	0.1098	0.0932	0.0098	0.9229	2880
1A-7_87	0.0208	0.0056	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3036	240
2A-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8580	0.0280	0.4755	720
2B-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3267	0.0027	0.1862	240
4B-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0046	0.0000	0.0913	90
3B-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3796	0.0028	0.2088	300
2A-15_89	0.0030	0.0000	0.0000	0.0000	0.0000	0.0064	0.0000	1.2304	0.0287	0.6663	2100
1B-4_89	0.0231	0.0025	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2346	90
2A-2_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1837	0.0000	0.1485	30
1C-12_89	0.0772	0.0157	0.0186	0.0000	0.0000	0.0087	0.0140	0.0069	0.0000	0.4250	720

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2A-14_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0066	0.0000	1.1315	0.0201	0.5285	1680
1A-16_89	0.2201	0.0828	0.0434	0.0326	0.0000	0.0246	0.0661	0.0816	0.0063	0.8438	2880
2B-18_87	0.0587	0.0000	0.0321	0.0000	0.0000	0.0277	0.0071	8.3696	0.7723	2.1943	4320
1B-2_89	0.0267	0.0040	0.0000	0.0000	0.0000	0.0034	0.0000	0.0000	0.0000	0.2327	30
4B-15_87	0.0758	0.0048	0.0093	0.0000	0.0000	0.0000	0.0000	0.4114	0.0062	0.7348	2130
3C-16_89	0.0260	0.0000	0.0094	0.0000	0.0000	0.0118	0.0032	1.5401	0.1358	0.7776	2880
3C-15_89	0.0124	0.0000	0.0000	0.0000	0.0000	0.0096	0.0029	1.2991	0.0944	0.5386	2100
4C-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0044	0.0000	0.0905	90
3A-1_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1756	0.0000	0.1630	1
1A-4_89	0.0217	0.0024	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2326	90
2A-19_87	0.0828	0.0026	0.0455	0.0077	0.0000	0.0423	0.0211	12.1421	1.3462	2.3400	4890
1B-3_89	0.0315	0.0041	0.0021	0.0000	0.0000	0.0037	0.0000	0.0029	0.0000	0.2271	60
1A-6_89	0.0414	0.0043	0.0067	0.0000	0.0000	0.0027	0.0045	0.0035	0.0000	0.2778	180
1B-4_89	0.0355	0.0046	0.0023	0.0000	0.0000	0.0000	0.0000	0.0025	0.0000	0.2467	90
2B-16_87	0.0102	0.0000	0.0070	0.0000	0.0000	0.0136	0.0000	3.9991	0.3358	1.2826	2880
4C-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0064	0.0000	0.0779	60
3B-13_89	0.0042	0.0000	0.0000	0.0000	0.0000	0.0084	0.0000	0.8685	0.0279	0.3555	1230
1A-1_89	0.0192	0.0021	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1858	1
3A-17_87	0.0088	0.0000	0.0000	0.0000	0.0000	0.0100	0.0000	2.1600	0.2389	1.4536	3540

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
1A-11_89	0.0702	0.0137	0.0104	0.0000	0.0000	0.0076	0.0098	0.0067	0.0000	0.3919	600
1A-2_89	0.0200	0.0040	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2240	30
3A-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6309	0.0131	0.4794	600
1B-17_89	0.4513	0.1966	0.1118	0.1056	0.0039	0.0459	0.1989	0.1809	0.0139	1.3714	3540
1B-12_89	0.0895	0.0320	0.0166	0.0046	0.0000	0.0124	0.0299	0.0131	0.0000	0.4446	720
2B-14_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0031	0.0000	1.1217	0.0128	0.5461	1680
3A-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2244	0.0020	0.1848	90
2B-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2572	0.0000	0.1509	60
2B-17_87	0.0242	0.0000	0.0178	0.0000	0.0000	0.0171	0.0000	5.1427	0.5129	1.5638	3540
4A-15_87	0.0110	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1374	0.0000	0.3473	2130
3B-17_89	0.0731	0.0017	0.0345	0.0047	0.0000	0.0282	0.0110	3.1059	0.3300	1.3150	3540
4A-16_87	0.0306	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2355	0.0000	0.4491	2880
1B-15_89	0.1892	0.0601	0.0427	0.0180	0.0000	0.0257	0.0502	0.0243	0.0000	0.7331	2130
4B-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0072	0.0000	0.0896	90
2A-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7575	0.0174	0.3606	360
1C-15_87	0.1730	0.0545	0.0305	0.0103	0.0000	0.0202	0.0541	0.0330	0.0048	0.8099	2120
1A-17_87	0.2943	0.1052	0.0557	0.0374	0.0000	0.0314	0.0965	0.0926	0.0069	1.2877	3530
2C-16_89	0.0351	0.0000	0.0157	0.0000	0.0000	0.0137	0.0041	1.9659	0.1440	0.8842	2880
3C-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3064	0.0024	0.2506	1

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
4A-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0021	0.0000	0.0795	30
4C-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0706	0.0000	0.2555	1680
1B-14_89	0.1197	0.0392	0.0235	0.0102	0.0000	0.0175	0.0437	0.0151	0.0000	0.5943	1680
1C-10_89	0.0608	0.0070	0.0108	0.0000	0.0000	0.0065	0.0069	0.0052	0.0000	0.3576	465
1A-5_89	0.0307	0.0022	0.0000	0.0000	0.0000	0.0039	0.0000	0.0000	0.0000	0.2469	120
1C-12_87	0.0783	0.0100	0.0117	0.0000	0.0000	0.0065	0.0120	0.0067	0.0024	0.4800	720
2A-18_89	0.1101	0.0052	0.0412	0.0123	0.0000	0.0387	0.0188	4.0327	0.3623	1.5827	4290
1A-6_87	0.0122	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2506	180
3A-15_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.3435	0.1260	0.9539	2130
3B-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6592	0.0111	0.5056	720
1A-19_87	1.1933	0.6699	0.3030	0.3097	0.1331	0.1348	0.5343	0.6489	0.0358	2.8739	4980
3A-18_87	0.0325	0.0000	0.0143	0.0000	0.0000	0.0192	0.0000	3.6643	0.4547	2.1516	4320
3B-17_87	0.0188	0.0000	0.0121	0.0000	0.0000	0.0155	0.0000	3.2731	0.3703	2.0466	3540
1A-1_87	0.0083	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2150	1
3C-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3826	0.0060	0.2978	30
2A-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6033	0.0000	0.2557	90
1C-4_87	0.0230	0.0042	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2515	90
3C-13_89	0.0023	0.0000	0.0000	0.0000	0.0000	0.0025	0.0000	0.8251	0.0378	0.3862	1230
4B-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0019	0.0000	0.0701	1

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3A-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9232	0.0629	0.6800	1290
1B-11_89	0.0570	0.0050	0.0127	0.0000	0.0000	0.0059	0.0086	0.0000	0.0000	0.3587	600
1C-14_89	0.1249	0.0299	0.0253	0.0000	0.0000	0.0202	0.0491	0.0159	0.0000	0.6066	1680
1C-5_89	0.0380	0.0046	0.0047	0.0000	0.0000	0.0048	0.0000	0.0000	0.0000	0.2413	120
4A-18_87	0.2713	0.0971	0.0317	0.0298	0.0000	0.0224	0.0161	0.9935	0.0917	1.4572	4320
1B-10_89	0.0503	0.0086	0.0083	0.0000	0.0000	0.0072	0.0068	0.0000	0.0000	0.3749	465
3C-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6042	0.0055	0.4614	720
1B-3_89	0.0357	0.0051	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2306	60
2A-15_89	0.0030	0.0000	0.0000	0.0000	0.0000	0.0073	0.0000	1.2784	0.0301	0.6545	2100
3C-18_89	0.0831	0.0031	0.0351	0.0074	0.0000	0.0310	0.0119	3.1240	0.3214	1.2654	4290
2B-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0041	0.0000	1.8880	0.0914	0.7718	1680
4A-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0089	0.0000	0.1058	240
3C-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2430	0.0018	0.1765	90
4A-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0069	0.0000	0.0764	60
2C-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2928	0.0000	0.1794	360
1C-14_87	0.1280	0.0352	0.0209	0.0082	0.0000	0.0166	0.0271	0.0257	0.0037	0.7191	1680
3B-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5098	0.0177	0.3730	240
2B-11_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4980	0.0127	0.2308	600
1A-11_87	0.0443	0.0088	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3924	600

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3C-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3738	0.0059	0.1946	360
2A-17_89	0.0394	0.0000	0.0201	0.0000	0.0000	0.0200	0.0094	2.3554	0.2080	1.2123	3560
3C-14_89	0.0127	0.0000	0.0024	0.0000	0.0000	0.0079	0.0000	1.0590	0.0610	0.4332	1680
2A-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8449	0.0134	0.4018	480
1C-1_89	0.0211	0.0022	0.0000	0.0000	0.0000	0.0036	0.0000	0.0000	0.0000	0.1941	1
4B-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0125	0.0000	0.1347	600
4B-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0054	0.0000	0.0823	30
1B-8_89	0.0428	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3170	300
1A-5_87	0.0260	0.0047	0.0000	0.0000	0.0000	0.0038	0.0000	0.0000	0.0000	0.2712	120
2B-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3669	0.0053	0.2357	465
1A-8_87	0.0282	0.0068	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3169	300
3B-18_87	0.0690	0.0036	0.0309	0.0042	0.0000	0.0330	0.0018	5.2111	0.6786	2.7444	4320
2B-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6582	0.0033	0.3489	240
3C-1_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1933	0.0000	0.1560	1
1C-6_89	0.0176	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2426	180
3C-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5153	0.0091	0.3807	300
2B-11_87	0.0000	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	1.0064	0.0293	0.4525	600
1A-14_89	0.1227	0.0229	0.0184	0.0000	0.0000	0.0120	0.0307	0.0133	0.0000	0.5283	1680
3A-13_89	0.0039	0.0000	0.0000	0.0000	0.0000	0.0080	0.0000	0.8679	0.0288	0.3634	1230

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2C-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2237	0.0000	0.1508	60
4B-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0199	0.0000	0.1164	480
4B-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0066	0.0000	0.1216	600
1A-3_87	0.0137	0.0034	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2734	60
4C-18_87	0.1376	0.0364	0.0168	0.0064	0.0000	0.0131	0.0028	0.6684	0.0366	1.1158	4320
3A-16_89	0.0296	0.0000	0.0092	0.0000	0.0000	0.0143	0.0040	2.0200	0.1726	0.8070	2880
4B-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0049	0.0000	0.0895	120
3A-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3657	0.0030	0.2048	240
1C-15_87	0.1645	0.0500	0.0302	0.0119	0.0000	0.0196	0.0282	0.0358	0.0000	0.7966	2120
1B-12_87	0.0590	0.0193	0.0145	0.0000	0.0000	0.0082	0.0044	0.0080	0.0023	0.4703	720
2A-15_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	2.2010	0.0910	0.8056	2130
2C-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4053	0.0052	0.2105	465
3C-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6163	0.0105	0.4610	720
3A-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6683	0.0067	0.4983	720
2A-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5475	0.0175	0.2634	30
2B-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2471	0.0000	0.2285	240
1C-9_87	0.0432	0.0079	0.0000	0.0000	0.0000	0.0062	0.0000	0.0000	0.0000	0.3399	360
2A-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2668	0.0000	0.1850	300
1A-7_89	0.0353	0.0042	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2834	240

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3C-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3648	0.0039	0.2167	360
3A-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3044	0.0000	0.2522	1
1A-1_89	0.0189	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1910	1
2C-16_87	0.0063	0.0000	0.0000	0.0000	0.0000	0.0099	0.0000	2.7114	0.2450	1.0719	2880
2C-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6090	0.0070	0.3309	300
3B-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6696	0.0079	0.5032	720
1B-6_87	0.0190	0.0027	0.0000	0.0000	0.0000	0.0027	0.0000	0.0000	0.0000	0.2758	180
4B-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0045	0.0000	0.0914	180
2B-16_89	0.0428	0.0000	0.0217	0.0000	0.0000	0.0175	0.0087	2.2123	0.1464	1.0267	2880
1B-8_89	0.0498	0.0077	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3235	300
3C-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4052	0.0079	0.3211	90
3B-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2617	0.0018	0.1842	120
2C-18_87	0.0418	0.0000	0.0219	0.0000	0.0000	0.0246	0.0122	8.6080	0.8063	1.9737	4320
4C-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0047	0.0000	0.0857	90
1B-13_87	0.0997	0.0193	0.0157	0.0022	0.0000	0.0111	0.0141	0.0197	0.0026	0.5985	1290
3C-19_87	0.1243	0.0061	0.0484	0.0143	0.0000	0.0434	0.0042	6.6541	0.9112	3.0416	5010
2B-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7375	0.0000	0.2932	180
2A-12_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0027	0.0000	0.5252	0.0137	0.2583	720
2C-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8951	0.0000	0.3635	480

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
4B-16_87	0.1442	0.0498	0.0160	0.0064	0.0000	0.0130	0.0030	0.6237	0.0485	1.0338	2880
4C-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0950	0.0000	0.2551	1680
3B-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4581	0.0000	0.2316	465
1A-7_89	0.0279	0.0049	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2700	240
3C-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5816	0.0057	0.4165	465
2B-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.9189	0.0096	0.5288	1230
1A-12_87	0.0625	0.0124	0.0079	0.0000	0.0000	0.0089	0.0065	0.0055	0.0000	0.4492	720
1C-12_87	0.0633	0.0078	0.0136	0.0000	0.0000	0.0067	0.0028	0.0059	0.0000	0.4720	720
2C-16_89	0.0309	0.0000	0.0155	0.0000	0.0000	0.0157	0.0000	1.9893	0.1447	0.8904	2880
2B-19_87	0.1365	0.0231	0.0645	0.0166	0.0000	0.0524	0.0367	13.0627	1.4098	2.6654	4890
2A-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3371	0.0022	0.1709	180
1C-6_87	0.0151	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2630	180
1B-14_89	0.1214	0.0291	0.0202	0.0097	0.0000	0.0170	0.0488	0.0228	0.0000	0.6121	1680
1C-16_87	0.2456	0.0914	0.0416	0.0250	0.0000	0.0271	0.0766	0.0568	0.0057	1.0317	2880
1A-17_89	0.2782	0.1191	0.0645	0.0438	0.0021	0.0285	0.1134	0.1314	0.0065	0.9931	3540
1B-18_89	3.9647	2.1909	0.9737	1.1887	0.6916	0.4448	2.0036	2.1971	0.5527	4.9949	4320
3A-15_89	0.0196	0.0000	0.0101	0.0000	0.0000	0.0108	0.0000	1.5693	0.0841	0.5741	2100
1A-10_89	0.0591	0.0072	0.0074	0.0000	0.0000	0.0062	0.0064	0.0000	0.0000	0.3566	465
2A-17_89	0.0573	0.0000	0.0273	0.0035	0.0000	0.0231	0.0107	2.8925	0.2576	1.1419	3560

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2C-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2527	0.0000	0.1589	90
2C-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3594	0.0000	0.2320	30
1B-7_89	0.0527	0.0057	0.0059	0.0000	0.0000	0.0058	0.0085	0.0033	0.0000	0.3120	240
3B-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2578	0.0021	0.1602	60
2B-15_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0077	0.0000	3.2192	0.1617	0.9489	2130
2A-2_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2670	0.0000	0.1373	30
1C-6_89	0.0338	0.0030	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2552	180
3B-2_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2441	0.0000	0.1645	30
2C-18_89	0.1663	0.0238	0.0701	0.0239	0.0000	0.0607	0.0323	5.1296	0.5097	1.7638	4290
4B-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0150	0.0000	0.1306	600
2A-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2642	0.0000	0.1382	60
4C-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0058	0.0000	0.1124	360
2C-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5567	0.0000	0.2525	60
1C-16_89	0.2508	0.0750	0.0558	0.0337	0.0000	0.0348	0.1079	0.0384	0.0000	0.8849	2880
2A-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	2.0785	0.0371	0.6758	1680
3A-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4334	0.0074	0.3134	90
2C-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7166	0.0000	0.2854	180
4A-16_87	0.0362	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2287	0.0000	0.4873	2880
2A-16_89	0.0219	0.0000	0.0042	0.0000	0.0000	0.0160	0.0000	2.2071	0.0975	0.8378	2880

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2A-12_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5490	0.0063	0.2572	720
2A-13_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8176	0.0204	0.3825	1230
1A-4_89	0.0331	0.0047	0.0051	0.0000	0.0000	0.0037	0.0036	0.0028	0.0000	0.2470	90
2C-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2521	0.0000	0.1495	60
2B-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0016	0.0000	0.2721	0.0000	0.1577	90
1B-18_87	0.3853	0.1635	0.0738	0.0513	0.0027	0.0408	0.1191	0.1745	0.0096	1.4365	4320
1A-8_87	0.0352	0.0060	0.0054	0.0000	0.0000	0.0052	0.0000	0.0027	0.0000	0.3315	300
1B-16_87	0.1833	0.0485	0.0267	0.0183	0.0000	0.0216	0.0150	0.0376	0.0055	0.8341	2880
1B-7_87	0.0238	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2929	240
2A-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7313	0.0094	0.3370	300
2A-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.7458	0.0241	0.5409	1230
2B-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2450	0.0000	0.1516	90
2C-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2826	0.0000	0.1564	180
4C-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0369	0.0000	0.1903	1230
2A-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.2485	0.0056	0.4088	720
3B-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5719	0.0085	0.4294	465
4A-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0112	0.0000	0.1015	240
3B-18_87	0.0700	0.0016	0.0261	0.0023	0.0000	0.0300	0.0051	5.1965	0.7109	2.7494	4320
3A-19_87	0.0506	0.0000	0.0217	0.0000	0.0000	0.0235	0.0000	4.4949	0.5884	2.5533	5010

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2C-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6250	0.0000	0.2606	60
1C-13_87	0.0657	0.0190	0.0163	0.0000	0.0000	0.0099	0.0038	0.0065	0.0000	0.5991	1290
4A-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0052	0.0000	0.0828	90
4A-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0154	0.0000	0.1389	720
3A-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2582	0.0022	0.1768	90
3A-18_89	0.0807	0.0039	0.0353	0.0092	0.0000	0.0347	0.0112	3.2939	0.3549	1.4046	4290
2C-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2307	0.0000	0.1694	240
3B-15_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.5320	0.1668	1.0966	2130
3A-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5080	0.0080	0.3758	240
1C-16_87	0.2440	0.0792	0.0406	0.0229	0.0000	0.0281	0.0832	0.0614	0.0066	1.0333	2880
3A-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3892	0.0049	0.2984	30
1B-17_87	0.2571	0.0896	0.0430	0.0364	0.0000	0.0276	0.0762	0.0579	0.0073	1.0617	3530
3A-19_87	0.0506	0.0000	0.0252	0.0000	0.0000	0.0255	0.0049	4.4649	0.5537	2.5626	5010
1B-9_87	0.0500	0.0056	0.0027	0.0000	0.0000	0.0062	0.0000	0.0029	0.0000	0.3454	360
1C-17_89	0.4246	0.2259	0.0902	0.1011	0.0068	0.0495	0.2028	0.1964	0.0120	1.3737	3540
2A-17_89	0.0541	0.0000	0.0242	0.0000	0.0000	0.0197	0.0098	2.3985	0.2003	1.2021	3560
2A-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5832	0.0039	0.2708	30
2A-16_87	0.0047	0.0000	0.0000	0.0000	0.0000	0.0083	0.0000	3.1046	0.1728	1.0714	2880
4A-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0210	0.0000	0.1378	600

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3A-11_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4485	0.0032	0.2582	600
1C-1_87	0.0136	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2172	1
1C-5_87	0.0159	0.0022	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2765	120
2C-14_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0029	0.0000	0.9842	0.0170	0.4874	1680
3A-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4200	0.0022	0.3083	60
3B-16_87	0.0079	0.0000	0.0000	0.0000	0.0000	0.0083	0.0000	2.1644	0.2379	1.4692	2880
3A-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3166	0.0050	0.1787	300
2A-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3366	0.0000	0.1610	90
1A-9_89	0.0691	0.0100	0.0085	0.0000	0.0000	0.0059	0.0000	0.0039	0.0000	0.3393	360
1B-3_87	0.0180	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2694	60
2C-14_89	0.0029	0.0000	0.0000	0.0000	0.0000	0.0053	0.0000	0.9519	0.0154	0.4988	1680
1A-12_89	0.0949	0.0359	0.0189	0.0079	0.0000	0.0114	0.0266	0.0331	0.0025	0.4444	720
2C-15_87	0.0020	0.0000	0.0000	0.0000	0.0000	0.0059	0.0000	2.4025	0.1158	0.8330	2130
2A-17_87	0.0182	0.0000	0.0134	0.0000	0.0000	0.0137	0.0000	3.7195	0.3367	1.4268	3540
1C-5_89	0.0391	0.0043	0.0022	0.0000	0.0000	0.0061	0.0028	0.0024	0.0000	0.2760	120
2C-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2870	0.0022	0.1797	120
4C-16_87	0.0183	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1786	0.0000	0.4335	2880
1A-17_89	0.2781	0.1178	0.0554	0.0341	0.0040	0.0291	0.1008	0.1187	0.0078	0.9754	3540
3A-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4331	0.0101	0.3126	90

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3B-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4415	0.0078	0.3291	120
3B-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5323	0.0130	0.4122	300
3B-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3966	0.0024	0.3205	60
1A-13_89	0.0782	0.0109	0.0120	0.0000	0.0000	0.0057	0.0229	0.0082	0.0000	0.5079	1290
3B-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2499	0.0022	0.1862	90
3A-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2828	0.0023	0.2509	1
1B-12_89	0.0943	0.0391	0.0198	0.0082	0.0000	0.0121	0.0294	0.0155	0.0023	0.4693	720
1B-16_89	0.3100	0.1252	0.0706	0.0549	0.0030	0.0328	0.1421	0.1145	0.0087	1.0873	2880
1C-12_87	0.0356	0.0105	0.0095	0.0000	0.0000	0.0077	0.0000	0.0000	0.0000	0.4125	720
3A-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3753	0.0052	0.3050	30
1C-13_89	0.1297	0.0407	0.0258	0.0085	0.0000	0.0143	0.0369	0.0375	0.0036	0.5700	1290
1B-5_89	0.0293	0.0047	0.0066	0.0000	0.0000	0.0030	0.0000	0.0000	0.0000	0.2683	120
1B-5_89	0.0373	0.0051	0.0048	0.0000	0.0000	0.0047	0.0000	0.0038	0.0000	0.2687	120
2B-18_87	0.0469	0.0000	0.0338	0.0000	0.0000	0.0294	0.0072	10.7489	1.1200	2.0308	4320
4C-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0692	1
1B-9_87	0.0471	0.0060	0.0071	0.0000	0.0000	0.0051	0.0000	0.0000	0.0000	0.3401	360
4A-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0038	0.0000	0.0747	1
3B-1_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2378	0.0000	0.1612	1
2C-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2323	0.0000	0.1546	90

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
1B-1_89	0.0214	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1935	1
1C-2_89	0.0363	0.0042	0.0039	0.0000	0.0000	0.0040	0.0035	0.0028	0.0000	0.2335	30
4C-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0045	0.0000	0.0744	30
1C-13_89	0.1420	0.0288	0.0251	0.0104	0.0000	0.0130	0.0349	0.0318	0.0000	0.5829	1290
3B-17_87	0.0200	0.0000	0.0133	0.0000	0.0000	0.0164	0.0000	3.2819	0.3854	2.0463	3540
2B-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8025	0.0149	0.3865	360
1C-3_87	0.0124	0.0017	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2618	60
4B-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0073	0.0000	0.1094	360
3B-11_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5336	0.0076	0.2399	600
2C-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2301	0.0000	0.1875	240
1B-14_89	0.1149	0.0464	0.0249	0.0100	0.0000	0.0178	0.0338	0.0103	0.0000	0.5771	1680
1A-4_87	0.0129	0.0033	0.0000	0.0000	0.0000	0.0000	0.0000	0.0016	0.0000	0.2879	90
2C-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7411	0.0138	0.3831	360
2B-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3160	0.0087	0.2191	360
2B-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.7064	0.0396	0.5915	1230
2B-16_89	0.0495	0.0000	0.0160	0.0000	0.0000	0.0165	0.0080	2.0016	0.1480	1.0486	2880
1C-15_89	0.1932	0.0687	0.0382	0.0159	0.0000	0.0211	0.0583	0.0518	0.0051	0.7335	2130
1B-1_89	0.0172	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1895	1
4B-15_87	0.0748	0.0050	0.0069	0.0000	0.0000	0.0077	0.0000	0.4145	0.0051	0.7319	2130

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
4A-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0039	0.0000	0.0698	1
3C-3_87	0.0017	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4319	0.0083	0.3250	60
1C-9_89	0.0458	0.0038	0.0097	0.0000	0.0000	0.0059	0.0000	0.0000	0.0000	0.3244	360
2A-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3511	0.0000	0.1803	240
3A-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5717	0.0093	0.4227	360
3B-12_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5756	0.0085	0.2597	720
3B-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3594	0.0000	0.2040	240
1C-14_89	0.1235	0.0345	0.0282	0.0155	0.0000	0.0168	0.0437	0.0181	0.0000	0.5892	1680
3A-5_89	0.0000	0.0000	0.0000	0.0000	0.0014	0.0000	0.0000	0.2455	0.0000	0.1835	120
2A-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3837	0.0000	0.1984	1
3A-17_87	0.0078	0.0000	0.0000	0.0000	0.0000	0.0102	0.0000	2.1649	0.2334	1.4489	3540
1A-19_89	0.6906	0.2897	0.1704	0.1691	0.0418	0.0754	0.2945	0.4403	0.0302	1.7499	5010
3C-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4309	0.0087	0.3231	60
4B-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0064	0.0000	0.0862	90
4B-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0052	0.0000	0.0965	180
2B-2_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2570	0.0000	0.1511	30
4C-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0099	0.0000	0.1285	720
3C-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3437	0.0052	0.2107	300
4B-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0041	0.0000	0.0829	30

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3A-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3643	0.0038	0.2030	240
2C-15_89	0.0069	0.0000	0.0000	0.0000	0.0000	0.0038	0.0000	1.3150	0.0394	0.6489	2100
1B-13_89	0.1454	0.0503	0.0273	0.0078	0.0000	0.0152	0.0323	0.0552	0.0037	0.5832	1290
2C-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.2893	0.0119	0.3725	600
3B-16_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0080	0.0000	2.1743	0.2187	1.4685	2880
4C-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0091	0.0000	0.1121	360
1C-14_87	0.1178	0.0463	0.0242	0.0083	0.0000	0.0169	0.0286	0.0297	0.0000	0.7248	1680
2C-13_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6766	0.0000	0.3327	1230
2C-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.9410	0.0503	0.6585	1680
1B-13_89	0.1307	0.0390	0.0300	0.0119	0.0000	0.0138	0.0248	0.0258	0.0000	0.5668	1290
2A-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8322	0.0214	0.3954	480
3A-2_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2135	0.0000	0.1643	30
3B-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4031	0.0144	0.3119	60
1A-5_87	0.0263	0.0044	0.0038	0.0000	0.0000	0.0038	0.0000	0.0000	0.0000	0.2744	120
1B-4_87	0.0130	0.0018	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015	0.0000	0.2828	90
4B-16_87	0.1417	0.0324	0.0157	0.0066	0.0000	0.0092	0.0033	0.6366	0.0365	1.0250	2880
2B-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8938	0.0000	0.3278	300
3B-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6903	0.0080	0.5005	720
3A-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4475	0.0053	0.3326	120

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
4C-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0049	0.0000	0.1181	480
4A-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0146	0.0000	0.1166	360
3B-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5281	0.0072	0.4136	300
2B-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2986	0.0000	0.1493	90
4B-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0460	0.0000	0.2001	1230
3C-17_89	0.0393	0.0000	0.0199	0.0000	0.0000	0.0179	0.0083	2.1633	0.1907	0.9354	3560
1C-10_89	0.0685	0.0073	0.0095	0.0000	0.0000	0.0067	0.0110	0.0048	0.0000	0.3758	465
3C-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3252	0.0027	0.2155	300
1A-13_89	0.1066	0.0119	0.0112	0.0000	0.0000	0.0119	0.0196	0.0000	0.0000	0.4514	1290
1C-8_87	0.0231	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3049	300
2C-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7115	0.0000	0.2648	120
2C-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6653	0.0000	0.3001	240
2A-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7383	0.0000	0.2776	180
4A-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0045	0.0000	0.0876	120
2C-12_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5736	0.0226	0.2718	720
1C-9_87	0.0201	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3062	360
1C-18_87	0.6689	0.3257	0.1499	0.1559	0.0291	0.0721	0.2126	0.3391	0.0216	2.4967	4320
1B-4_87	0.0123	0.0027	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2845	90
3C-17_87	0.0178	0.0000	0.0109	0.0000	0.0000	0.0137	0.0000	2.8358	0.3229	1.8159	3540

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3C-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9610	0.0670	0.6935	1290
4C-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0036	0.0000	0.0769	30
1B-10_87	0.0466	0.0068	0.0069	0.0000	0.0000	0.0061	0.0000	0.0000	0.0000	0.3572	495
1A-14_89	0.0896	0.0197	0.0171	0.0000	0.0000	0.0114	0.0263	0.0091	0.0000	0.5205	1680
2A-11_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0026	0.0000	0.5036	0.0077	0.2482	600
3B-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3232	0.0061	0.2555	1
2B-16_87	0.0147	0.0000	0.0000	0.0000	0.0000	0.0113	0.0000	5.4191	0.3125	1.2228	2880
3A-4_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2639	0.0027	0.1789	90
2A-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5838	0.0000	0.2602	60
3A-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5388	0.0127	0.4048	300
1A-8_87	0.0213	0.0038	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3119	300
2B-1_89	0.0000	0.0000	0.0000	0.0000	0.0156	0.0000	0.0000	0.2038	0.0000	0.1405	1
1B-4_89	0.0337	0.0047	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2383	90
3A-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3023	0.0000	0.2072	180
3B-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2241	0.0020	0.1684	60
2B-14_89	0.0029	0.0000	0.0000	0.0000	0.0000	0.0035	0.0000	1.1222	0.0205	0.5591	1680
1C-7_89	0.0261	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2664	240
1C-13_87	0.0841	0.0141	0.0110	0.0000	0.0000	0.0134	0.0040	0.0062	0.0000	0.5948	1290
1A-5_87	0.0173	0.0027	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2574	120

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3A-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5685	0.0098	0.4374	465
3C-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.1164	0.0600	0.7828	1680
2C-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4275	0.0000	0.2398	30
4A-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0250	0.0000	0.1412	600
2C-17_89	0.0611	0.0000	0.0239	0.0037	0.0000	0.0256	0.0100	2.7090	0.2069	1.2871	3560
2C-13_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6890	0.0000	0.3291	1230
3C-19_89	0.1510	0.0258	0.0577	0.0191	0.0000	0.0535	0.0256	5.0299	0.5599	1.7690	4830
1C-15_89	0.1894	0.0511	0.0384	0.0172	0.0000	0.0216	0.0646	0.0336	0.0053	0.7309	2130
1C-5_87	0.0157	0.0041	0.0000	0.0000	0.0000	0.0021	0.0000	0.0018	0.0000	0.2852	120
1B-15_89	0.2034	0.0595	0.0396	0.0246	0.0000	0.0219	0.0585	0.0625	0.0072	0.7814	2130
2A-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3861	0.0000	0.2014	1
2A-15_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	2.8007	0.0864	0.7671	2130
1A-18_87	0.3775	0.2247	0.0887	0.0838	0.0095	0.0474	0.1289	0.1379	0.0085	2.0329	4320
1C-16_89	0.2499	0.0891	0.0605	0.0334	0.0000	0.0321	0.1194	0.0575	0.0129	0.8835	2880
1C-4_89	0.0203	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2263	90
1B-8_87	0.0230	0.0038	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2999	300
2C-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6481	0.0108	0.3232	300
1A-14_89	0.1372	0.0435	0.0296	0.0118	0.0000	0.0155	0.0359	0.0232	0.0043	0.5942	1680
2C-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7059	0.0000	0.2557	120

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3B-12_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0030	0.0000	0.4936	0.0165	0.2980	720
3A-16_89	0.0335	0.0000	0.0122	0.0000	0.0000	0.0145	0.0000	2.0388	0.1939	0.8175	2880
3A-12_89	0.0013	0.0000	0.0000	0.0000	0.0000	0.0029	0.0000	0.5379	0.0078	0.3007	720
1C-19_87	1.8918	1.2157	0.4936	0.5494	0.2511	0.2122	0.9328	1.2481	0.1540	3.5732	4980
3B-17_89	0.0772	0.0031	0.0332	0.0035	0.0000	0.0305	0.0107	2.9645	0.3223	1.3396	3540
3B-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0023	0.0000	1.2921	0.1310	0.8974	1680
2C-12_87	0.0019	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.1270	0.0392	0.4689	720
3A-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6411	0.0125	0.4779	600
1C-10_87	0.0374	0.0039	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3649	495
2C-19_87	0.0617	0.0017	0.0348	0.0062	0.0017	0.0337	0.0084	8.3297	0.8250	2.2700	4890
1B-9_87	0.0173	0.0035	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3242	360
2C-17_87	0.0069	0.0000	0.0093	0.0000	0.0000	0.0148	0.0000	4.7272	0.3928	1.3700	3540
1C-18_89	1.0352	0.5493	0.2462	0.2873	0.1173	0.1160	0.4490	0.7114	0.0953	2.5581	4320
4B-15_87	0.0791	0.0047	0.0099	0.0000	0.0000	0.0063	0.0020	0.4210	0.0099	0.7307	2130
1C-1_89	0.0203	0.0016	0.0000	0.0000	0.0000	0.0020	0.0000	0.0000	0.0000	0.2108	1
2B-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5159	0.0000	0.2559	60
2B-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9349	0.0000	0.3619	360
4C-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0070	0.0000	0.1274	600
3A-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3182	0.0031	0.1987	180

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
1B-17_89	0.4794	0.1991	0.1067	0.0990	0.0072	0.0548	0.2080	0.1511	0.0193	1.2762	3540
1B-13_89	0.1546	0.0542	0.0289	0.0180	0.0000	0.0150	0.0466	0.0502	0.0037	0.5859	1290
3B-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.2702	0.0965	0.8958	1680
2C-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.4728	0.0064	0.5250	1230
3A-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9586	0.0451	0.6815	1290
3A-12_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5719	0.0106	0.2725	720
3C-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3495	0.0028	0.1969	240
1B-18_89	4.1729	2.4176	1.1242	1.2645	0.7797	0.4782	2.2246	2.6845	0.5651	4.7676	4320
3A-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2676	0.0024	0.1973	120
1A-18_89	0.4007	0.1908	0.0913	0.0869	0.0121	0.0430	0.1494	0.2254	0.0085	1.2764	4320
2A-3_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2553	0.0000	0.1339	60
2A-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4587	0.0030	0.2071	465
2A-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5726	0.0178	0.2527	30
2A-1_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3225	0.0000	0.1904	1
3A-15_89	0.0147	0.0000	0.0075	0.0000	0.0000	0.0100	0.0000	1.3427	0.0796	0.6001	2100
1C-18_87	0.7173	0.3408	0.1620	0.1718	0.0532	0.0788	0.2767	0.3730	0.0260	2.4117	4320
1C-6_87	0.0276	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2750	180
1A-11_87	0.0683	0.0087	0.0074	0.0000	0.0000	0.0084	0.0057	0.0047	0.0000	0.4155	600
1C-2_89	0.0264	0.0039	0.0041	0.0000	0.0000	0.0036	0.0000	0.0028	0.0000	0.2332	30

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
4A-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0092	0.0000	0.0950	180
2C-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2533	0.0000	0.1593	240
2A-15_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	2.4709	0.0788	0.7824	2130
1A-19_87	1.1189	0.6801	0.2783	0.2798	0.0879	0.1253	0.4522	0.6119	0.0388	2.9802	4980
2B-18_89	0.1482	0.0167	0.0610	0.0164	0.0000	0.0527	0.0279	5.1685	0.4780	1.7067	4290
1C-15_87	0.1537	0.0643	0.0344	0.0104	0.0000	0.0173	0.0323	0.0404	0.0056	0.7920	2120
1A-17_87	0.3411	0.1140	0.0639	0.0468	0.0000	0.0348	0.1055	0.0732	0.0000	1.2028	3530
3C-18_87	0.0372	0.0000	0.0161	0.0000	0.0000	0.0220	0.0000	4.2042	0.4931	2.4309	4320
4C-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0086	0.0000	0.1157	480
2C-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.9283	0.0418	0.6729	1680
1B-6_87	0.0224	0.0048	0.0000	0.0000	0.0000	0.0038	0.0000	0.0000	0.0000	0.2868	180
3B-18_89	0.1484	0.0205	0.0622	0.0183	0.0000	0.0548	0.0301	5.2959	0.6242	1.6695	4290
2A-1_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2062	0.0000	0.1342	1
1A-3_87	0.0165	0.0036	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2753	60
3C-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5201	0.0045	0.4054	360
1C-17_89	0.4525	0.2234	0.1205	0.0979	0.0150	0.0539	0.2107	0.2403	0.0108	1.4118	3540
4B-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0062	0.0000	0.0931	240
3C-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4382	0.0067	0.3211	90
4B-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0045	0.0000	0.0855	60

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
1C-5_87	0.0140	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2607	120
3C-12_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0014	0.0000	0.5139	0.0043	0.2480	720
3B-14_89	0.0124	0.0000	0.0090	0.0000	0.0000	0.0085	0.0000	1.1817	0.0724	0.4759	1680
2A-18_89	0.1088	0.0135	0.0437	0.0134	0.0000	0.0376	0.0256	4.3649	0.3914	1.5469	4290
3C-2_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2067	0.0000	0.1589	30
2C-10_87	0.0000	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000	0.8797	0.0108	0.3708	480
1A-9_87	0.0146	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3277	360
2B-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9551	0.0000	0.3162	240
3A-2_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2014	0.0000	0.1665	30
4C-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0070	0.0000	0.1124	480
1B-10_87	0.0268	0.0045	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3436	495
3B-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3640	0.0022	0.2856	30
2A-7_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3459	0.0024	0.1672	240
1A-6_87	0.0192	0.0036	0.0000	0.0000	0.0000	0.0025	0.0000	0.0000	0.0000	0.2874	180
3B-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5881	0.0061	0.4428	360
2C-5_87	0.0000	0.0021	0.0000	0.0000	0.0000	0.0000	0.0000	0.6099	0.0035	0.2736	120
1A-5_89	0.0396	0.0052	0.0051	0.0000	0.0000	0.0042	0.0000	0.0000	0.0000	0.2571	120
2B-11_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4715	0.0080	0.2346	600
3C-15_89	0.0091	0.0000	0.0031	0.0000	0.0000	0.0106	0.0000	1.4481	0.0668	0.5241	2100

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
1C-7_89	0.0505	0.0060	0.0035	0.0000	0.0000	0.0030	0.0056	0.0038	0.0000	0.3042	240
2C-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7289	0.0000	0.2903	180
4A-4_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0064	0.0000	0.0894	90
2C-15_89	0.0047	0.0000	0.0000	0.0000	0.0000	0.0068	0.0000	1.1158	0.0329	0.6762	2100
3B-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0383	0.0450	0.7343	1290
1A-9_89	0.0612	0.0065	0.0092	0.0000	0.0000	0.0059	0.0050	0.0050	0.0049	0.3270	360
1A-2_89	0.0238	0.0020	0.0000	0.0000	0.0000	0.0039	0.0000	0.0000	0.0000	0.2244	30
3C-6_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3180	0.0053	0.1831	180
3B-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4276	0.0098	0.3375	120
1B-6_89	0.0502	0.0061	0.0098	0.0000	0.0000	0.0045	0.0086	0.0053	0.0000	0.2982	180
3C-2_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4015	0.0054	0.3044	30
1A-15_89	0.1490	0.0575	0.0311	0.0101	0.0000	0.0164	0.0377	0.0368	0.0047	0.6432	2130
3B-15_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.5572	0.1538	1.0863	2130
4A-5_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0049	0.0000	0.0886	120
1A-12_89	0.0722	0.0143	0.0113	0.0044	0.0000	0.0120	0.0127	0.0060	0.0000	0.4277	720
4C-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0058	0.0000	0.1021	300
2A-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8080	0.0195	0.3565	360
2B-13_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8315	0.0142	0.4249	1230
2B-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9362	0.0263	0.4542	600

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2B-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3259	0.0022	0.2179	300
4C-15_87	0.0102	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1076	0.0000	0.3347	2130
3C-10_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4421	0.0068	0.2112	465
3C-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5710	0.0023	0.4277	465
2A-5_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2892	0.0025	0.1796	120
4A-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0219	0.0000	0.1330	480
2C-8_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2678	0.0000	0.1632	300
3C-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3798	0.0000	0.2198	360
2B-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8885	0.0101	0.3762	360
3C-16_87	0.0073	0.0000	0.0000	0.0000	0.0000	0.0043	0.0000	2.0472	0.2118	1.4017	2880
3A-1_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2146	0.0018	0.1597	1
3A-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6784	0.0064	0.5046	720
3B-15_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0024	0.0000	1.5726	0.1558	1.0883	2130
2B-15_89	0.0032	0.0000	0.0000	0.0000	0.0000	0.0076	0.0000	1.3602	0.0263	0.6726	2100
1B-11_89	0.0782	0.0152	0.0120	0.0000	0.0000	0.0074	0.0250	0.0087	0.0000	0.4264	600
2C-15_89	0.0046	0.0000	0.0000	0.0000	0.0000	0.0038	0.0000	1.3544	0.0339	0.6406	2100
2A-6_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7265	0.0000	0.2774	180
4C-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0028	0.0000	0.1033	240
1B-5_87	0.0246	0.0051	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2529	120

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
2B-15_87	0.0075	0.0000	0.0000	0.0000	0.0000	0.0095	0.0000	2.8355	0.1657	0.9992	2130
3C-17_89	0.0375	0.0000	0.0157	0.0000	0.0000	0.0165	0.0000	1.8740	0.1770	0.9661	3560
4B-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0052	0.0000	0.1046	240
2B-9_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3067	0.0022	0.2204	360
1B-14_87	0.1005	0.0223	0.0184	0.0032	0.0000	0.0165	0.0189	0.0074	0.0000	0.6315	1680
3B-18_89	0.1093	0.0217	0.0545	0.0185	0.0000	0.0507	0.0233	4.5975	0.5231	1.7471	4290
3C-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6094	0.0079	0.4616	600
2B-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	2.6895	0.0631	0.6870	1680
2A-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.4880	0.0081	0.5533	1230
2A-14_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	2.0393	0.0693	0.6885	1680
2B-2_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2341	0.0000	0.1522	30
1B-18_87	0.3615	0.1903	0.0795	0.0673	0.0042	0.0424	0.1261	0.1869	0.0081	1.4749	4320
3B-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5853	0.0092	0.4303	465
4C-7_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0058	0.0000	0.0910	240
1C-9_87	0.0259	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.3188	360
2B-12_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5203	0.0082	0.2512	720
1A-4_89	0.0341	0.0055	0.0024	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2406	90
1B-18_87	0.3756	0.1771	0.0726	0.0549	0.0000	0.0413	0.1361	0.1519	0.0100	1.3988	4320
1A-4_87	0.0181	0.0046	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015	0.0000	0.2976	90

Sample	Heavy arom C	Heavy arom D	Heavy arom E	Heavy arom F	Heavy arom G	Heavy arom H	Heavy arom I	Heavy monoaromatics A	Heavy monoaromatics B	Naphthalene	Weathering Time (min)
3B-1_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1963	0.0021	0.1674	1
1A-12_87	0.0551	0.0097	0.0051	0.0000	0.0000	0.0069	0.0000	0.0000	0.0000	0.4196	720
2B-11_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0346	0.0223	0.4451	600
3A-9_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5447	0.0082	0.4094	360
4A-10_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0187	0.0000	0.1303	480
4B-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0096	0.0000	0.1274	720
4A-13_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0322	0.0000	0.2275	1230
3C-12_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6099	0.0067	0.4578	720
2C-17_89	0.0558	0.0000	0.0278	0.0033	0.0000	0.0228	0.0103	2.6511	0.2184	1.3111	3560
3A-3_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.4213	0.0042	0.3102	60
3C-17_89	0.0439	0.0000	0.0111	0.0000	0.0000	0.0166	0.0040	1.9713	0.1837	0.9554	3560
2B-1_89	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2378	0.0000	0.1300	1
4A-8_87	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0132	0.0000	0.1109	300
1A-16_89	0.2161	0.0870	0.0457	0.0241	0.0000	0.0237	0.0854	0.0901	0.0057	0.8490	2880