

A Stable Isotope Stratigraphy of the Axel Heiberg Fossil Forest and its Application to Eocene Climate

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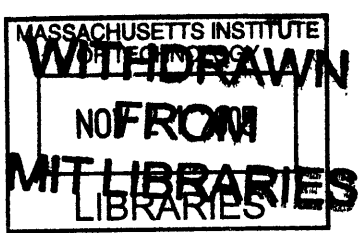
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LINDGREN

ABSTRACT

The Eocene era was a warm, climatically dynamic transitional period between the Paleocene greenhouse world and the Oligocene icehouse world. This study details carbon and hydrogen isotopic and biomarker analyses of samples of lignite (bulk fossil leaves), wood, paleosol, and resinite from the Middle to Late Eocene age fossil forest stratigraphy on Axel Heiberg Island, Nunavut, Canada.

Bulk carbon isotopes show a record of frequent, large fluctuations on the scale of the Paleocene-Eocene Thermal Maximum benthic carbon excursion of $\sim 2.6\text{‰}$ (Zachos 1999). However, terrestrial flora are less sensitive to CO_2 fluctuations given their capacity to regulate stomatal intake and the comparatively easy diffusion of CO_2 in air. Resinites ($-22.8 \pm 1.7\text{‰}$) are enriched relative to bulk lignite ($-24.7 \pm 0.75\text{‰}$), and wood ($-21.66 \pm 0.45\text{‰}$) is also enriched relative to bulk lignite. Both 1) a scenario of periodic methane hydrate pulses and 2) a scenario of fluctuating forest stand LAI (leaf area index) are not inconsistent with our data. Either mechanism could be responsible for large carbon isotope shifts.

Higher plant input dominated the *n*-alkane signature. Compound-specific hydrogen isotopes in *n*-alkanes show a record of marked secular change, with isotopes becoming generally lighter over the time span of the stratigraphy, though punctuated by singular fluctuations as large as 32‰ . Polycyclic isoprenoid lipids (-266‰ to -375‰ , mean $300\text{‰} \pm 38\text{‰}$) are characteristically depleted relative to *n*-alkanes (-238‰ to -295‰ , mean $-268\text{‰} \pm 10\text{‰}$). From the *n*-alkanes, we estimate that environmental water in the Eocene on Axel Heiberg Island was depleted $-150\text{‰} \pm 24.8\text{‰}$, which agrees with an estimate derived from cellulose, $\delta\text{D}_{\text{environmental}} = -133\text{‰}$ (Jahren 2003). (For comparison, modern precipitation at the site has a δD value of $\sim -213\text{‰}$, though precipitation should not be considered equivalent to environmental water.) This datum is consistent with a meridional weather patterns that may have carried moisture over continents towards high latitudes in the absence of a polar front, isotopically depleting precipitation to a greater extent than occurs today. However, seasonality cannot be discounted as a mechanism, given that colder temperatures would lead to colder condensation temperatures and thus, isotopically lighter precipitation.

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II. Introduction

The Eocene

The Eocene era began with the Paleocene-Eocene Thermal Maximum (54.8 Ma), an event defined by a global spike in temperature and a dramatic carbon isotope excursion, as recorded in benthic foraminifera (Zachos 2001). Throughout the rest of the Eocene, global mean temperatures generally became cooler. The Eocene-Oligocene boundary at 33.7 Ma marked the onset of permanent glacier formation in Antarctica (Zachos 2001). These two boundaries are well-studied, being sharply defined in the proxy records by oxygen isotopes (Fricke 1998, Ivany 2000), carbon isotopes (Katz 1999, Norris 1999) coupled oxygen and carbon isotopes (Bolle 200a, Bolle 200b, Diester-Haas 1996, Thomas 2002), coupled carbon and sulfur isotopes (Kurtz 2003), barium isotopes (Bains 2000), strontium isotopes (Brewster-Wingard 1997), osmium isotopes (Ravizza 2003), extraterrestrial ^3He (Farley 1998, 2003), Mg/Ca ratios (Billups 2003, Bolle 2001 clay, Brewster-Wingard 1997, Tripathi 2004), Sr/Ca ratios (Sarangi 2001), dinoflagellate extinction (Crouch 2001), clay minerals (Robert 1997, Murru 2003) and pedogenic carbonates (Sarkar 2003, Schulz 2002, Segall 2000, Sheldon 2002).

However, fewer studies are available on the Middle Eocene, or Lutetian Age, from 49-41.3 Ma. Available evidence indicates that the era was characterized by an exotic climate regime that allowed for warm temperatures above the Arctic Circle. High-latitude mean annual temperature (MAT), inferred from fossil palms on Axel Heiberg and Ellesmere Islands (the landmasses closest to the geographical North Pole), was about 8.2-9.3°C at sea level, near the coasts (Greenwood 1995). This estimate is based on the Nearest Living Relative (NLR) approach, which assumes that the palm species of the era

had similar tolerances to frost as their present-day nearest living relatives. Fossils from sites in interior North America, South America, Asia, Antarctica and Australia also show evidence that temperatures in the continental interiors did not drop below freezing, or at least, not for an appreciable amount of time (Greenwood 1995).

This warm climate hypothesis is further supported by evidence from the Axel Heiberg fossil forest. In the Eocene, this site lay well above the Arctic Circle. All data indicate the existence of a flourishing, warm-temperate swamp-forest. The preserved tree stumps exhibit an unusual lack of late wood in their growth rings. This could indicate a lack of hardening, a physiological response to frost (Basinger 1991). Faunal evidence also indicates a warm and equable climate in high latitudes, based on a macrofossil vertebrate assemblage from Axel Heiberg Island that includes turtles and champsosaurs, a crocodile-like reptile (Tarduno 1998, Eberle 1999).

Global mid-Eocene climate can be characterized as “spatially equable,” in two ways. Both the 1) equator-to-pole temperature gradient and the 2) continental coast-to-interior gradient were much reduced. Both aspects are discussed below.

1) In the Eocene Arctic, estimate of the Cold Month Mean (CMM) are 2.0°C ; estimate of MAT is 8.2°C (Greenwood 1995). From the equator to the poles, then, MATs spanned only ~ 8 to 30°C across the hemispheres for a net gradient of 22°C^1 . For comparison, today’s equator-to-pole gradient is approximately -22 to 28°C , for a net gradient of 50°C (all data in Greenwood 1995). Commonly called the “greenhouse world,” the Eocene earth was most likely kept warm by greenhouse gases: water vapor,

¹ Most estimates of tropical Eocene SST published before 2001 relied on foraminiferal data that indicated far cooler temperatures. However, these estimates have since been shown to result from poor preservation (Pearson 2001). Greenwood’s study relied on terrestrial NLR data, so was impervious to this particular bias.

methane and/or carbon dioxide. From Axel Heiberg Island, cellulose studies yielded an estimate of twice the amount of water vapor present in the atmosphere today; this water vapor could have contributed to keeping the poles warm (Jahren 2003). Additionally, data exist to support methanogenesis in Arctic soils, as evidenced by unusually enriched calcium carbonate in permineralized fossil tree stumps (Jahren 2004). This methane could have also contributed to the greenhouse effect.

These gases alone, however, do not explain the decrease in thermal gradient. They only explain the increase in overall temperature: greenhouse gases simply amplify what already exists. The decrease in gradient can be explained only by an alteration in heat transport from the tropics, the “sun belt” that receives the bulk of Earth’s insolation. From the tropics, there are two possible carriers of heat: the ocean and the atmosphere. However, in this scenario, the atmosphere lacks both the strength and longevity necessary to produce a lasting effect on high latitudes. It is possible that intensified cyclonic activity in the tropics caused deeper vertical mixing in the ocean, which, in turn, transported a greater proportion of heat to high latitudes, where it could warm the poles (Emanuel 2001). The poles were warm for approximately ten million years (Zachos 1994), and the mechanism responsible for this sustained warmth has been a topic of much debate. Increased CH₄ levels may have led to the formation of polar stratospheric clouds, which would have kept the poles warm (Kirk-Davidoff 2002). However, efforts at modeling sustained methane emissions have failed to produce this effect (Korty, pers. comm.).

2) Not only was the equator-to-pole temperature gradient reduced, but the temperature gradient from coast to continental interior was also unusually slight. Abundant evidence exists for warm continental interiors in Australia and North America,

with CMM up to 10°C, from palm assemblages (Greenwood 1995) and faunal assemblages (Wing 1991). Climate modelers have long tried to account for this unusual finding. The temperatures of continental interiors do not usually mirror those of their coasts; a moist column of air tends to dry out and lose heat along its trajectory over land. Though the question remains largely unresolved, invocation of realistic orbital parameters (Sloan 1998), incorporation of a full annual cycle of SST values (Sloan 2001), introduction of high-latitude vegetation feedback (Upchurch 1998), and models that include reduced obliquity (Sewall 2004) have done much to reconcile models with proxy data. According to Sloan (1998), in the best-fit models, wind on Axel Heiberg Island was either nonexistent or strong from the northeast. Either scenario would have strong implications for precipitation provenance.

However, the gradients may be even more dramatic than the estimate from NLR studies. Royer (2002) studied long-term (two-year) frost tolerances of several species used as NLRs under high CO₂, including the palms used in Greenwood (1995). The study concluded that palms freeze more easily, i.e. at warmer temperatures from +0.6°C to +3.7°C, under elevated CO₂ levels. The effect in springtime, when trees manufacture the bulk of their tissue, is an average of 1.1°C greater than the effect in fall. As a result, estimates of the cold month mean temperature (CMM) in NLR studies may undershoot by at least 1.5°C to 3.0°C. Gross morphological characteristics of these palms have remained constant in time (Wing and Greenwood 1993). However, it is not known whether *response* to elevated CO₂ levels has remained constant in individual taxa since the Cretaceous. Nevertheless, errors of +/- 3.0°C should be applied to estimates of CMM.

This could mean that the sea-level temperature on Axel Heiberg Island was as much as 12.3°C in the Eocene (Greenwood 1995, Royer 2003).

Seasonality, or annual temperature cyclicality, on the other hand, remains pronounced in the available records. Therefore, based on these studies, Eocene climate may have been spatially equable, but was not *temporally* equable. Mean annual temperature range (MART), as deduced by carbon and oxygen isotopes in Paris basin² *Turritella* shells, show evidence of seasonality indistinguishable from that of today, except that the mean annual temperature was ten degrees higher (Andreasson 1996). Axel Heiberg Island and the Paris Basin are geographically displaced, so these data are of limited value, though we should also consider them given the absence of a polar front and the spatially equable climate.

Several recent studies have illustrated the dynamism of Eocene climate, of echoes of the extremes that mark its beginning and end. Western North Atlantic Middle Eocene foraminifera show >1‰ variability in $\delta^{18}\text{O}$ on thousand-year timescales, which, given the magnitude of a shift expected from modest sea ice formation, was attributed to fluctuations in SST (Wade 2002). (1‰ of $\delta^{18}\text{O}$ change is equivalent to ca. 4°C of water temperature change.)

Several studies analyzing planktonic foraminifera have noted tropical sea surface temperatures paradoxically *cooler* than present (e.g. Savin 1977, Shackleton 1981, Bralower 1995). However, later work by Kobashi (2001) hypothesized that these cool readings may have been due to a shift in plankton blooms to wintertime, where they recorded cooler temperatures. Mollusk shells from the same time period record warm

² The Paris Basin is located in modern-day north central France.

temperatures consistent with all other proxy and model data (Kobashi 2001). However, it is now believed that the cold bias was simply due to diagenetic alteration and poor preservation (Pearson 2001).

Pearson (2000) and Bohaty (2003) noted evidence of large CO₂ volcanic outgassing events in the Early Eocene, and lack of evidence for any Middle to Late Eocene events. In contrast, this period of CO₂ pulses also featured a sharp rise of +1‰ in benthic δ¹⁸O, an isotopic event that may indicate transient continental ice. (For isotopic enrichment of benthic foraminifera to occur, bottom waters must cool or continental ice volume must increase, because isotopically light precipitation is sequestered in the ice sheets.) This implies that ice sheets were forming far earlier than the Eocene-Oligocene Boundary, when permanent ice sheets were established in Antarctica (Zachos 1999).

Throughout the Eocene, from 50-32 Ma, there are huge fluctuations in Calcite Compensation Depth, or CCD (the depth at which rate of dissolution exceeds rate of deposition, and below which no carbonate is deposited). At 47 Ma, at the approximate time of our stratigraphy, the percent of carbonate being deposited in tropical equatorial Pacific and subtropical south Atlantic sediments was extremely low; therefore the CCD was extremely shallow (Tripathi 2005). CCD is directly related to ocean acidity, which in turn is directly related to atmospheric pCO₂. A shallow CCD indicates high pCO₂.

The same records showed that positive δ¹⁸O excursions and sea level lowstands occurred during rapid CCD deepening. If deep CCD coincides with low pCO₂, this is consistent with the other two data, which indicate transient continental ice sheets. However, studies from Mg/Ca ratios in foraminifera suggest that ice volume could have

been no more than 25% of modern ice volume any time during the Eocene (Billups and Schrag 2003).

Overall, studies show an incredibly dynamic transition from the Paleocene greenhouse world to the Oligocene icehouse world. This transitional time is known as the Eocene.

The Fossil Forest on Axel Heiberg Island

Axel Heiberg Island lies above the Arctic Circle at 74°N, a maximum of 6° from its position in the Eocene (Irving 1991) (Figure 1).

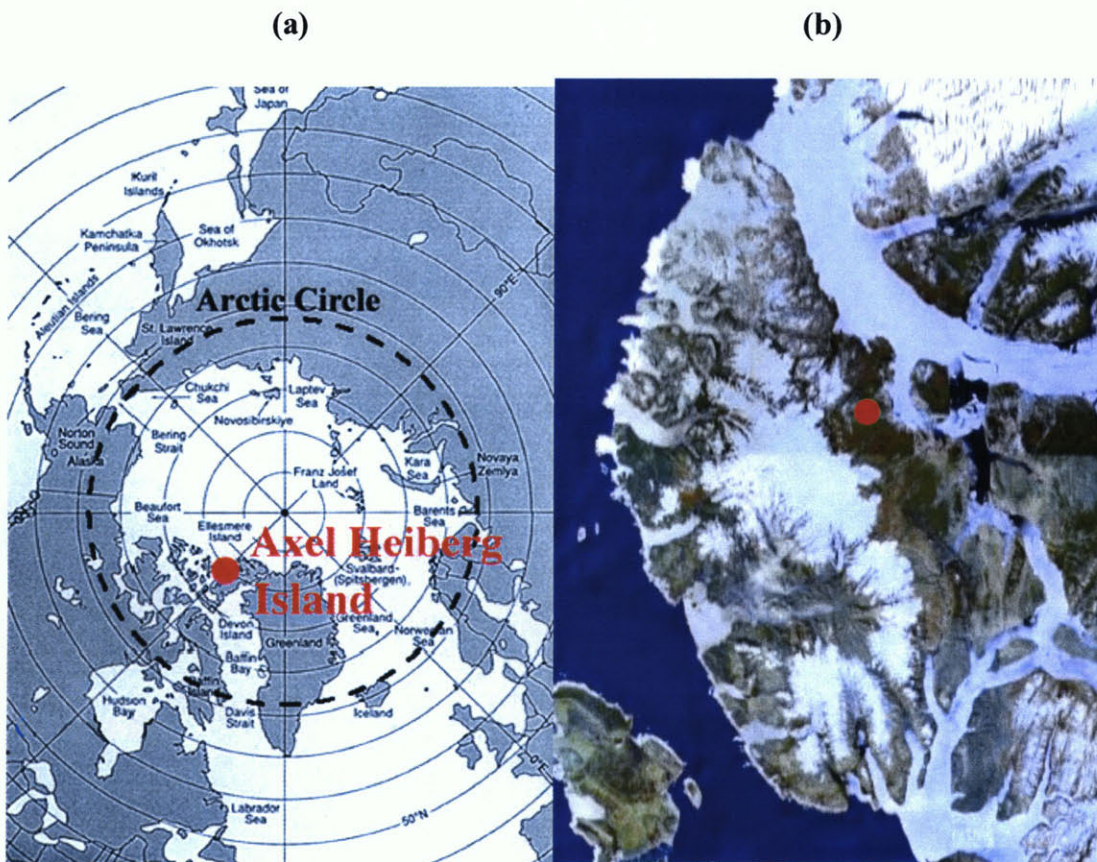


Figure 1. a) Map showing the present-day location of Axel Heiberg Island. Map from Jahren and Sternberg (2002), *GSA Today*. Used with permission. b) Satellite image of present-day Axel Heiberg Island, with fossil forest site highlighted with red dot. Image courtesy © Google Maps.

On this island, there is an extraordinarily well-preserved stratigraphy of temperate floodplain forests at 79°55N to 79°59N (Eberle 1999). The most widely accepted age for the fossil forest is Middle to Late Eocene (Jahren and Sternberg 2002), based on vertebrate fossils found in a syndepositional formation on westward Ellesmere Island (Dawson 1976). However, because of non-temporally-specific pollen and plant macrofossil assemblages (McIntyre 1991), a time window extending from the Early Eocene to the Early Oligocene cannot be discounted.

The stratigraphy is contained within the Buchanan Lake Formation, the youngest unit of the Eureka Sound Group. Composed of lithic sandstone, mudstone, siltstone and lignite, this unit formed as a result of local tectonic activity (LePage and Basinger 1991), uplifting the Princess Margaret Arch to the west (Eberle 1999), which produced diabase-rich sediment in alluvial fans upon which the forest developed (Ricketts 1991). Late Cenozoic and Quaternary erosion then exposed the stratigraphy (LePage and Basinger 1991).

The Fossil Forest sequence comprises a total of 120 meters, a distance of 10-18 kilometers from the once-eroding orogeny (Jahren and Sternberg 2002, Ricketts 1991). The area featured braidplains and meanderplains with water channels that frequently shifted (Ricketts 1991). Organic productivity is estimated to have been $\sim 1200 \text{ g/m}^2/\text{year}$, with 325-484 stumps per hectare. This is comparable to Alabama cypress swamps (169 stumps/hectare), tropical rainforests (200-1000) and Finland spruce forests (485). Rainfall is estimated to have been 100-150 cm annually (MacIntyre 1991), compared to only 0.65 cm today (Tarnocai 1991). Floral input, as deduced from macrofossil

assemblages (Basinger 1991), did not undergo major changes over the depositional time span. However, MacIntyre (1991) asserts that the pollen assemblages tell a story of a dynamic, constantly changing floodplain environment where forest was not always the dominant ecosystem.

The most abundant foliage is widely regarded to be that of *Metasequoia* (Francis 1991), though this assumption is brought into question by the assertion that most of the unassociated resinites found on Axel Heiberg were synthesized by *Pseudolarix* (Anderson 1995). Modern *Metasequoia* is intolerant of both shade and intense light, and grows best on open soils (Vann 2005). Given that *Metasequoia* has remained at least morphologically static since the Cretaceous, we might assume that the floodplain swamp featured growing conditions of medium light intensity and open soils, conducive to *Metasequoia*'s growth.

The deciduous nature of *Metasequoia* remains a mystery. It was long believed that *Metasequoia* evolved to shed its leaves annually because of polar winter, which comprises three months of total darkness (Spicer 1990). This assumes that the amount of respired carbon during times of darkness would exceed the amount of carbon lost through simply dropping the leaves altogether, and growing new ones come spring. However, Royer (2003) showed that *Metasequoia* loses an order of magnitude more carbon via leaf abscission than its closely-related evergreen counterpart, *Sequoia sempervirens*, does through wintertime respiration. Further results suggested that deciduous trees increase their rates of photosynthesis proportional to their carbon loss, resulting in a net primary productivity (NPP) comparable to that of evergreens. However, the root cause of *Metasequoia*'s deciduousness remains unknown.

The excellent preservation of the fossils in the Buchanan Lake Formation is indicated by several factors. First, the fossils are plainly recognizable. Tree stumps, logs, leaves, seed cones, and fruits can be identified. They are only dried, and slightly to heavily compressed (Jahren 2004). Second, the preservation of cutin acids, labile biomolecules that degrade easily during early diagenesis, indicates good preservation (Stankiewicz 1997), as does the presence of intact chloroplasts (Schoenhut 2005). Permineralization of tree stumps is low to nonexistent (Grattan 1991).

It is widely believed that the individual fossil forest layers were buried in episodic, massive flood events that enabled plant material to be mummified in shallow, anoxic, reducing waters (Yang 2004). This argument is supported by the presence of lepidocrocite, a secondary soil mineral indicative of a periodically reducing environment, is found in the site's paleosols, along with other characteristics associated with hydromorphic soils (Jahren 2004). Finally, Eberle (1999) noted the absence of bone material in the layers, another indicator of an acidifying environment.

Biomarkers: *an overview*

Resilient biomolecules, derived from ancient organisms and preserved through time, serve as paleoproxies for climatic and other parameters. If their primary structural characteristics can remain chemically stable during early diagenesis and later burial, they can encode information in three ways.

1) First, a lipid's *structure* can be diagnostic of the metabolic pathway used to synthesize it. For example, acetogenic lipids (e.g. *n*-alkanes) and isoprenoid lipids (e.g. hopanoids) use C₂ and C₅ building blocks, respectively (Hayes 2001).

2) Second, a lipid's *structure* can be diagnostic of the organisms themselves. For example, predominance of *n*-alkanes of chain length under 18 are diagnostic of bacteria; chain lengths over 25 are diagnostic of higher plant input (Sachse 2004).

3) Third, a lipid's *isotopic* signature can be diagnostic of the source material, i.e. snow vs. rainwater, or the partial pressure of atmospheric carbon dioxide. This applies if isotope effects associated with the pathway and organism are known (Sessions 1999, Sauer 2001).

Yang (2005) analyzed pyrolysates of Middle Eocene leaves from Ellesmere Island and identified lignins, polysaccharides, and alkyls. The presence of polysaccharides in a 45 Ma leaf sample indicates the excellent degree of preservation. The presence of lignin, the tough polymer of wood, is less surprising. Alkyls comprise a relatively small proportion of the total pyrolysate.

Biomarkers: *n*-alkanes

N-alkane lipids, a major focus of this study, are built from acetate precursors. After biosynthesis in the plastid and excretion through the endoplasmic reticulum, they are excreted immediately to the leaf surface. There, they form essential components of plant cuticular waxes, whose functions include protection against ultraviolet radiation, protection from water saturation, and restriction of water loss (Kunst 2003). Variation in saturated *n*-alkane chain length may indicate any of three known signals: *in vivo* precursor (Figure 2), source organism (Figure 3), or source plant component (e.g. leaf versus wood). Other effects on *n*-alkane chain length, discussed below, include latitude, temperature, precipitation and insolation.

N-alkanes found in the fossil record are derived from acetogenic precursors as seen in Figure 2. With the exception of *n*-alkanes (i.e. *n*-alkanes synthesized as such, and not derived from any precursor) and wax esters³, chain length ranges in plants fall between ~20-35 carbons.

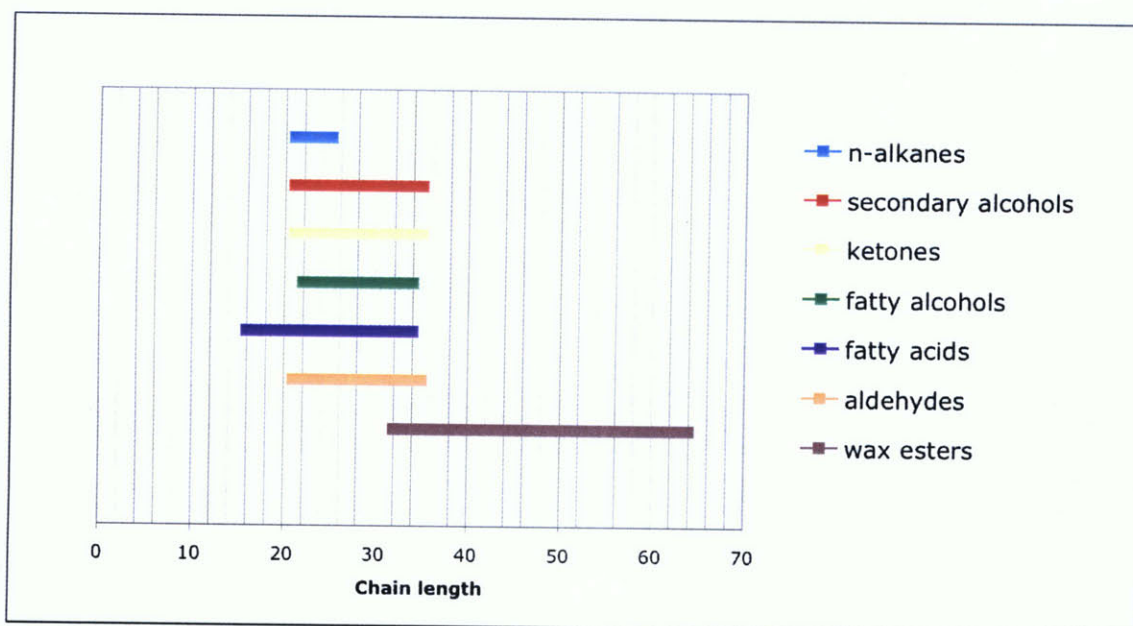


Figure 2. Chain length ranges of wax classes in plants. Data compiled in Kunst (2003).

Variation in *n*-alkane chain length is also indicative of the source organism (Figure 3). Short *n*-alkanes (C_{12} to C_{22} all) are characteristic of algae and photosynthetic bacteria. Even-numbered, short *n*-alkanes (C_{12} to C_{22} even) are characteristic of bacteria (Sachse 2004). C_{21} - C_{25} odd *n*-alkanes are characteristic of submerged aquatic plants (Ficken 2000). The leaf waxes of higher plants are longer, in range of C_{25} - C_{31} (odd), and

³ Wax esters are made by linking fatty acids and fatty alcohols via the acyl reduction pathway, which explains why their length is approximately double that of a single fatty acid or fatty alcohol (Kunst 2003).

beyond (Sachse 2004). *Sphagnum* moss, a common input to peat bogs, exhibits distinctive C₂₃, C₂₅ and C₃₁ dominances (Baas 2000).

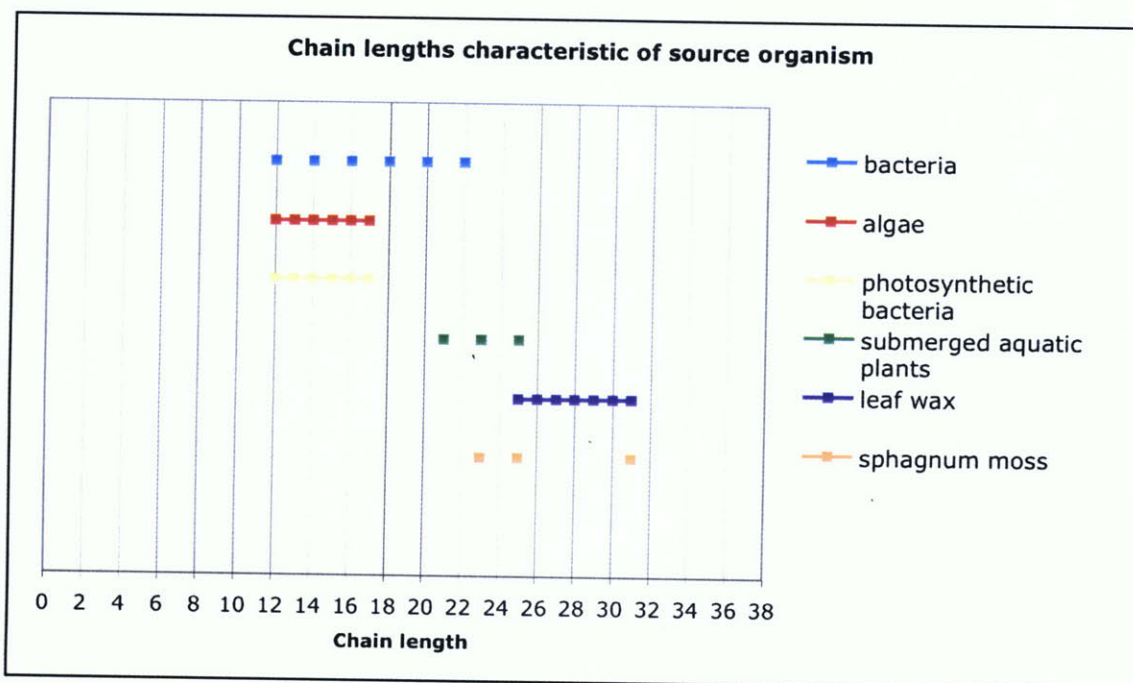


Figure 3. For *n*-alkanes, chain length is characteristic of the source organism. Data compiled in Sachse 2004. Note that the values listed for submerged aquatic plants is derived from a limited study of four modern lacustrine environments (Ficken 2000). *Sphagnum* is a taxon of moss common to peat deposits (Baas 2000).

N-alkane chain length can also vary depending on the plant component being studied. For example, via pyrolysis chromatography, Yang (2005) found that *n*-alkanes derived from modern *Metasequoia* leaf surfaces were dominated by C₂₅ whole-leaf pyrolysates were dominated by C₂₉.

In one study, average *n*-alkane chain length (ACL) increased along a longitudinal transect towards the equator (Sachse 2005b). The author suggests that as temperatures

warm, chain lengths lengthen and thus cuticular wax becomes more dense, so as to protect against excess evapotranspiration. However, other mechanisms may be involved.

It is important to note, first, that cuticular wax occurs as amorphous crystalloids on the leaf surface (Kunst 2003); thus the *n*-alkanes will pack in an ordered, lengthwise fashion. (This excludes the possibility that longer chain lengths lead to looser packing.)

Greater pCO₂ in lower latitudes, or in warmer climes, could contribute to accelerated rates of photosynthesis, thereby making more carbon available for lipid synthesis. In fact, pCO₂ has been shown to be the primary forcing on photosynthetic rate, which also increases as relative humidity levels approach 70% (Vann 2005). Given that relative humidity for Middle Eocene Axel Heiberg was estimated to be 67% (Jahren 2003), it is possible that photosynthetic rates were relatively high, enabling higher rates of biosynthesis and thus longer-chain *n*-alkanes. Thicker wax could also protect against greater precipitation by expelling rain droplets, or against greater ultraviolet radiation in regions of greater insolation (Kunst 2003). Further data are necessary to understand the nature of this trend.

In situ, the distribution of *n*-alkane lengths in leaves is strongly even over odd, given that *n*-alkanes' precursors are made by adding two carbons at a time, from acetate. In very recent depositions, the distribution is roughly bell-shaped. In fossils, however, the distribution flips to an odd-over-even abundance. This is due to decarboxylation, or the loss of one terminal carbon, in early diagenesis (Staccioli 2002).

Biomarkers: *isoprenoids*

Isoprenoid lipids have a far greater range of structural variation, given that isoprene units are made up of five nonlinear carbons. They are also characteristically depleted in deuterium compared to biomass (-212‰ to -303‰) and to *n*-alkanes (-60‰ to -112‰) (Chikaraishi 2004b). Isoprenoids are made by one of two pathways: the mevalonic-acid (MEP) pathway in the chloroplast, and the non-mevalonic-acid (MVA) pathway in the cytosol (Hayes 2001). Both have characteristic isotope effects. The MEP pathway, which produces C₂₀ isoprenoids, has a greater depletive effect (-283‰ to -303‰) than the MVP pathway, which produces C₁₅ and C₃₀ isoprenoids (-212‰ to -283‰). If a mixture of individual isoprenoids is cross-plotted according to hydrogen and carbon isotopes, clumping occurs, and the provenance of each can be clearly distinguished (Chikaraishi 2004b). However, the reason for the hydrogen isotopic difference between the MEP and MVP pathways is still unknown (Sessions 1999).

Biomarkers: *hydrogen isotopes*

Hydrogen isotopes in lipids can indicate the isotopic composition of source water, and/or prevailing climatic conditions such as relative humidity. The lipids in this study were extracted from four distinct sources: organic-rich lignites, wood fragments, resinates, and associated paleosols. The lipids in these different materials manifest the source water signature differently.

δD of lipids is controlled by three factors, as outlined in Sessions (1999):

- 1) δD of the biosynthetic precursors, i.e. acetate or isoprene,
- 2) fractionation and exchange during the biosynthetic process, and

3) hydrogenation from NADPH during biosynthesis.

NADPH is made by either of two processes: electron transport chains in photosynthesis, or sugar oxidation in the pentose-phosphate pathway in the cytosol. Given that these occur separately in the chloroplast and cytosol, respectively, NADPH cannot be treated as a single, isotopically uniform pool (Sessions 1999).

Each of the materials will now be considered separately.

1) The lignites studied here are made up largely of leaf and forest floor detritus. The lipids therefore will represent water that has come straight from root to stem to leaf, but are slightly enriched due to evapotranspiration effects. The lignites may also represent accumulated aquatic plant material, given that these forests existed in floodplain and swamp environs (Eberle 1999).

2) Wood is composed of sclerenchyma fibers and tracheids, dead cells that hardens to form xylem, the channel that transports water up from roots. There are two principal macromolecular components of wood.

Cellulose, the most abundant component, is synthesized in the presence of stem water, such that its leaf-derived isotopic signal is erased. It has been estimated that 32% and 42% of hydrogen and oxygen, respectively, is exchanged with the stem water (Roden and Ehleringer 1999). However, it is possible to study only the non-exchangeable hydrogen in cellulose, as demonstrated by Jahren and Sternberg (2003).

Lignin, on the other hand, is the tough, hydrophobic, chemically complex polymer that makes up the bulk of xylem cells (Campbell 1999). Gymnosperms are distinguished by a G-lignin, made from monomers of coniferyl alcohol, a product of

ferulic acid (Savidge 2001). The biosynthesis of lignin is an extremely complex process, and poorly understood (Onnerud 2002). Therefore, whatever hydrogen signal it may manifest is not likely to have a straightforward interpretation.

3) Resin is the sap that fills in wounds caused by predators, physical damage, or as a defense against pathogens (Anderson and Crelling 1995). Most relevant to this study, it is also produced during periods of sudden growth, i.e. the early spring growing season, as a stopgap in expanding wood (Jahren 2002). In *Metasequoia*, as in all members of the warm-temperate *Taxodiaceae* family, constitutive resin occurs in the leaves, while induced resin occurs in the wood. These two functional types of resin may have different compositions, though that information is not currently known (Anderson and Crelling 1995).

All resinites have a polymeric component, which is highly conserved, and a monomeric component, which is widely variable across fossil and recent resinites (Anderson and Crelling 1995). Class I resinite is characteristic of gymnosperms. It is also chemically distinct; its monomeric component is labdanoid diterpane (C_{20}) (Figure 5).

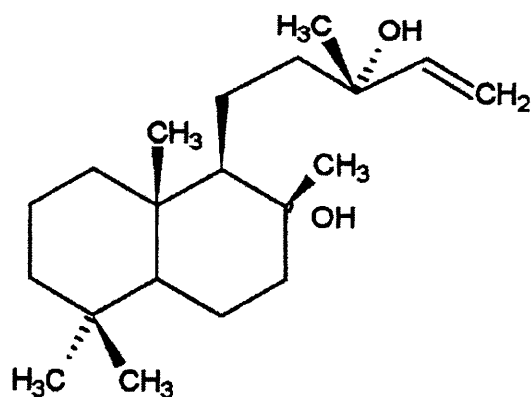


Figure 5. A C_{20} labdane, the basic monomer of Class I resinites. Structure credit: Mendoza 2002.

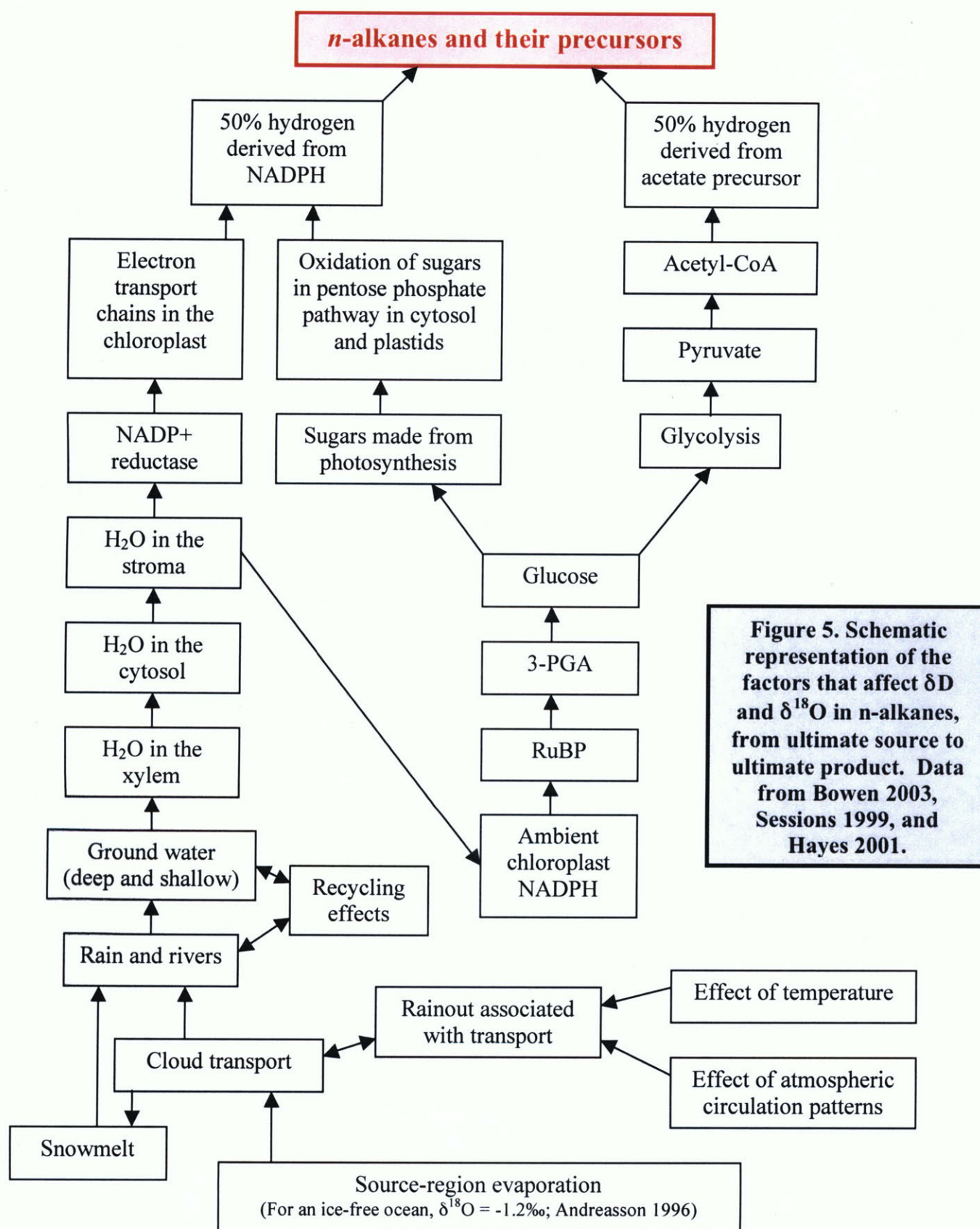
4) Paleosols are the organic-poor, mineral-rich soils found associated with the tree stumps. The mineral matrix could feature enriched isotopes, the complement to depleted organic matter (e.g. Jahren 2004). The lipids found therein, however, may come from soil-dwelling bacteria, or simply the same sources as lignites, having been merely deposited into another matrix. Therefore the δD values are of little value.

The δD values of lipids are, in part, controlled by the isotopic composition of the environmental water, which is in turn comprised in part by meteoric water. So, while δD values of lipids cannot be directly attributed to δD of precipitation, it is an important factor to consider.

The δD value of meteoric water is affected by three processes: source-region evaporation, rainout associated with transport, and recycling effects at the site of deposition. In general, rain becomes more depleted from equator to poles, from coasts to continental interiors, and at high elevations, because of slightly lower vapor pressure for isotopically depleted water (Bowen 2003).

The Global Meteoric Water Line (GMWL) describes the linear relationship between oxygen and hydrogen isotopes in precipitation. The modern equation is $\delta D = 8\delta^{18}O + 10$ (Craig 1961). Interestingly, Jahren (2003) observed a highly linear relationship between δD and $\delta^{18}O$ isotopes in the cellulose with a slope of 9.5 ± 2 , differing from the modern GMWL. This may indicate an Eocene era local GMWL on Axel Heiberg Island (Jahren 2003), or it may indicate fractionation processes unique to the Axel Heiberg Island ecosystem.

These hydrological factors are combined with those that govern H and O isotopic fractionation during lipid biosynthesis (Sessions 1999, Hayes 2001) as shown in Figures 5 (acetogenic synthesis) and 6 (isoprenoid synthesis).



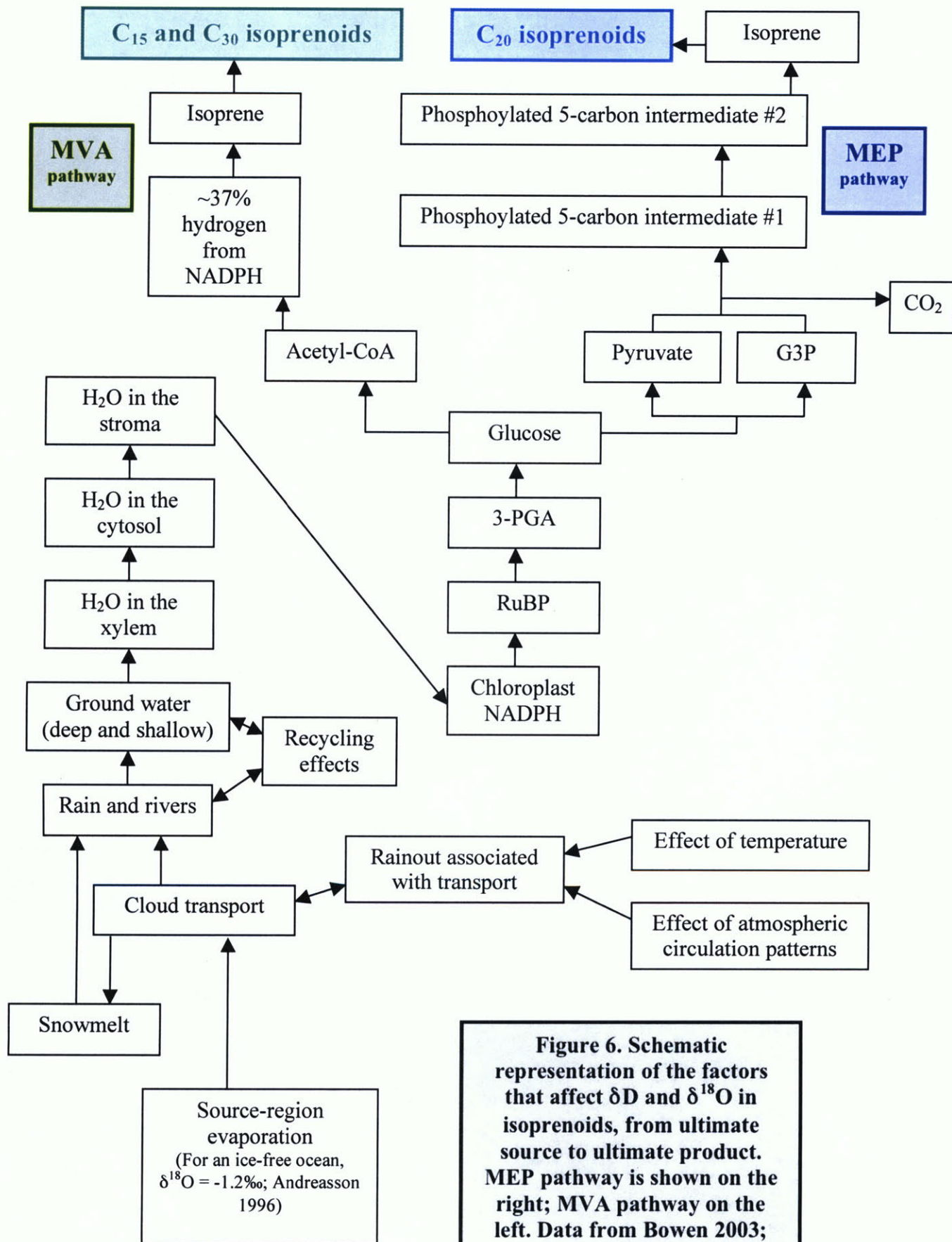


Figure 6. Schematic representation of the factors that affect δD and $\delta^{18}O$ in isoprenoids, from ultimate source to ultimate product. MEP pathway is shown on the right; MVA pathway on the left. Data from Bowen 2003; Chikaraishi 2003, 2004a, 2004b; Sessions 1999, and

The isotopic discrepancy between *n*-alkanes and isoprenoids is uniformly observed in the literature (Sauer 2001, Hayes 2001, Sessions 1999, Chikaraishi 2003, 2004a, 2004b). *N*-alkanes are synthesized in the plastid (Kunst 2003), with $\epsilon_{\text{alkane/water}} = 91\text{-}152\text{‰}$. MVP isoprenoids are synthesized in the cytosol (Hayes 2001), with $\epsilon_{\text{alkane/water}} = 212\text{-}238\text{‰}$. MEP isoprenoids are synthesized in the chloroplast, with $\epsilon_{\text{alkane/water}} = 238\text{-}303\text{‰}$ ($\epsilon_{\text{alkane/water}}$ data from Chikaraishi 2004b; “water” refers to ambient, or growth, water). Either the three biosynthetic pathways have different isotope effects, or the initial pools of hydrogen in each compartment have different isotope ratios. In reality, both of these factors probably contribute. In the acetogenic pathway, the four-carbon metabolic intermediate undergoes keto-enol tautomerization. That is, a hydrogen atom – from isotopically heavy cell water – attaches, thereby contributing to the final *n*-alkyl product, making up as much as 75% of its bound hydrogens (Chikaraishi 2004b, Sessions 2002).

Carbon Isotopes

Carbon isotopes of plants, and individual components of plants, indicate the degree to which the leaves of that plant discriminated against ^{13}C during gas exchange with ambient air (Dawson 2002) and during biosynthetic processes (Hayes 2001). Today’s post-industrial atmospheric CO_2 has been isotopically depleted by the burning of fossil fuels, and now has $\delta^{13}\text{C}$ averaging $\sim -8\text{‰}$, an increase in depletion from pre-industrial levels of $\sim -6.4\text{‰}$ (Broadmeadow and Griffiths 1993). Today’s C_3 plants average, by bulk, -26‰ (Kelly 1998). As a general rule, when atmospheric pCO_2 increases, $^{13}\text{C}_{\text{plant}}$ decreases (Grocke 2002). This may make intuitive sense: when there is more carbon in the air, the leaves would discriminate against ^{13}C to a greater extent,

resulting in more depleted biomass. However, as Arens (2000) pointed out after amassing 517 data points of $p\text{CO}_2$ vs. $\delta^{13}\text{C}_{\text{plant}}$ over 176 species, there is no significant correlation between the two variables when the unique contribution of $\delta^{13}\text{C}_{\text{atmosphere}}$ is excluded. Therefore, increased $p\text{CO}_2$ does not in itself cause greater depletion. Rather, when $p\text{CO}_2$ increases, the new carbon is usually isotopically light. That is, the primary control on $\delta^{13}\text{C}_{\text{plant}}$ is $\delta^{13}\text{C}_{\text{atmosphere}}$. This may explain the relationship observed by Grocke (2002) and others.

Farquhar (1989) determined an equation that allows for calculation of $\delta^{13}\text{C}_{\text{atmosphere}}$ from the parameters a (fractionation caused by the diffusion of air, 0.0044), b (fractionation caused by carboxylation, 0.027), p_i (the partial pressure of atmospheric carbon dioxide within the leaf) and p_a (the partial pressure of atmospheric carbon dioxide surrounding the leaf). a and b represent kinetic fractionation factors. p_i/p_a is controlled by ecological factors, such as relative humidity, drought stress, growth form, and soil salinity (Arens 2000).

$$\delta^{13}\text{C}_{\text{air}} = \delta^{13}\text{C}_{\text{plant}} + a + (b-a)(p_i/p_a) \quad (1)$$

Plugging in the aforementioned values of a and b , and a characteristic C3 value for p_i/p_a of 0.7 (after Grocke 2002), the above equation simplifies to:

$$\delta^{13}\text{C}_{\text{air}} = \delta^{13}\text{C}_{\text{plant}} + 20.22 \quad (2)$$

Note that p_i/p_a can change because of environmental factors such as nutrient and water deprivation or low light levels (Arens 2000). However, given that there is ample floral evidence that our paleoenvironment suffered no lack of water or nutrients (Ricketts 1991, Francis 1991, Basinger 1991), we would assume $p_i/p_a = 0.7$. Note also that as $p\text{CO}_2$ increases, a plant keeps its ratio of intracellular to extracellular carbon dioxide constant (Beerling 1996).

However, this equation assumes that $p\text{CO}_2$ is the primary forcing on plant ^{13}C fractionation. As elucidated above, the majority of changes in $\delta^{13}\text{C}_{\text{plant}}$ can be attributed to changes in $\delta^{13}\text{C}_{\text{atmosphere}}$ rather than changes in $p\text{CO}_2$ (Arens 2000), with R^2 correlation values of 0.97 and 0.002, respectively. A new equation arises from this result:

$$\delta^{13}\text{C}_{\text{CO}_2} = (\delta^{13}\text{C}_{\text{plant}} + 18.67)/1.10 \quad (3)$$

This equation was used to predict both modern $\delta^{13}\text{C}_{\text{atm}}$ and Holocene $\delta^{13}\text{C}_{\text{atm}}$. Both predictions agreed well with modern data and proxy records, respectively, demonstrating the robustness of the equation.

Again, the four materials studied here may manifest the atmospheric carbon isotope signal differently. Because lignites are mainly leaf detritus, these will record a $\delta^{13}\text{C}$ value closest to $\delta^{13}\text{C}_{\text{atm}}$, and we will use the lignites to extrapolate Eocene $\delta^{13}\text{C}_{\text{atmosphere}}$ using Equation (3). The atmospheric signals given by bulk wood, resin and paleosols are probably too complex to untangle, especially in the absence of compound-specific isotope information. Paleosols have been used as a paleobarometer for the

Holocene (e.g. Kelly 1998); far more intimate knowledge of soil formation is required for such analysis than is available for these Eocene sediments.

However, other workers have studied pedogenic carbonates, as well as additional proxies for pCO₂ in the Middle Eocene. Authors, estimates, methods and applicable caveats are summarized in Table 1. Note: pre-industrial value was ~280 ppmv; modern, post-industrial value is ~365 ppmv (Keeling and Whorf 1998).

Authors	pCO₂ Estimate	Proxy
Ekart <i>et al.</i> (1999)	900 ppmv	pCO ₂ barometer in paleosols
Pearson and Palmer (2000)	2000 ppmv	Boron isotopes in calcite shells
Royer <i>et al.</i> (2001)	320 ppmv	Stomatal indices
Berner and Kothavala (2001)	700 ppmv	GEOCARB II model
Retallack (2001)	1600-2000 ppmv	Stomatal indices
Yapp (2004)	2700 +/- 300 ppmv	Pedogenic goethite

Table 1. Listing of previous estimates of Eocene pCO₂ by various proxies.

As the data in Table 1 show, there is a huge range of estimated values for Eocene pCO₂ – from 320 ppmv (close to modern value) to 3000 ppmv – based on the approach used. The average of all estimates is 1400 +/- 900 ppmv.

Ekart *et al.* (1999) estimate pCO₂ levels to be 900 ppmv; however, the paleobarometer approach assumes $\delta^{13}\text{C}_{\text{atm}}$, $\delta^{13}\text{C}_{\text{soil}}$, and soil respiration rate. The estimate of Pearson and Palmer (2000) relies upon assumptions of ancient $\delta^{11}\text{B}_{\text{seawater}}$, alkalinity and ΣCO_2 . Berner and Kothavala (2001) modeled Middle Eocene pCO₂ levels with GEOCARB III, though the time resolution of this model is only 10 Ma, with linear extrapolation in between. Retallack (2001) estimated pCO₂ levels from stomatal indices, though the study employed only one taxon, *Ginkgo*. Yapp (2004) estimated Eocene pCO₂ levels using pedogenic goethite, but the estimate applies to the Early Eocene only. Royer *et al.* (2001) also estimated pCO₂ levels with stomatal indices. His estimate of ~300 ppmv is near modern levels, with the assumption that stomata have the same relationship to pCO₂ levels as they do now. This seems the safest assumption, though the fact that its resultant estimate is so significantly lower than that from all the other proxies casts it in doubt.

Very few studies have looked at the carbon isotopes of resinites, either in bulk or compound-specific, though the work of Anderson and Crelling (1995) and Murray (1998) has partially addressed this. The average bulk $\delta^{13}\text{C}$ of modern Class I resinite is -25.8 +/- 1.5‰, while values of Tertiary Class I resins (those resins characteristic of gymnosperms) are -22.8 +/- 1.7‰ (Murray 1998). The carbon isotope values of resinites serve as a foil for those of leaves, given that resinites are composed of C₂₀ polylabdanoids made by the highly depletive MEP pathway.

Opal Phytoliths

Opal phytoliths are silica particles that accumulate within plants over a wide range of taxa, especially grasses, which mold them in their own shapes. In marine records, phytoliths serve as proxies of wind strength. However, in terrestrial records they serve as proxies of the dominant vegetation, e.g. C3 or C4 grasses. These data, in turn, offer climatic information. C3 grasses dominate in cooler, moist climates; C4 grasses dominate in warm, sunny, arid climates (Abrantes 2003).

In the Axel Heiberg fossil forest horizons, there exist marked white layers that were investigated by Tarnocai (1991) and Foscolos (1991). Unfortunately, burial and subsequent dehydration caused the phytoliths to dehydrate into amorphous silica, thereby losing all identifying structural characteristics (Tarnocai 1991).

The Scope of this Study

This paper will analyze data from samples collected over the entire Axel Heiberg Fossil Forest stratigraphy. The data manifest in four major categories:

- 1) biomarker structures, both acetogenic and isoprenoid;
- 2) *n*-alkane abundances, absolute and relative;
- 3) compound-specific D/H isotope ratios of biomarkers; and
- 4) bulk $^{13}\text{C}/^{12}\text{C}$ isotope ratios.

With these data, this paper will address the magnitude, frequency and possible mechanisms of Middle Eocene climate variability at high latitudes.

III. Experimental

Sample Collection and Transport

The entire fossil forest stratigraphy, which encompasses 120 meters of sediment (Ricketts 1991), is shown in Figure 7.

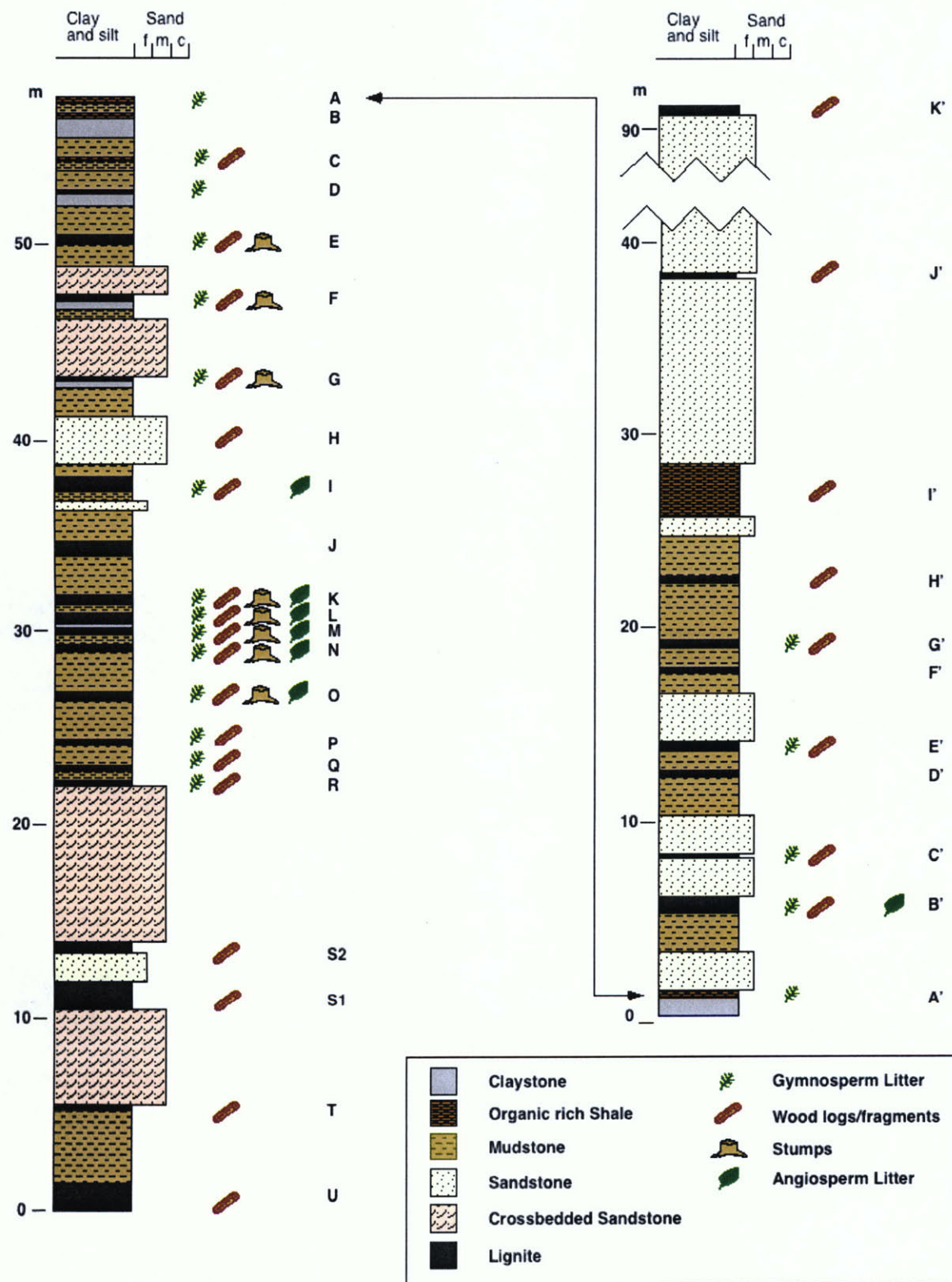


Figure 7. The Axel Heiberg Island fossil forest stratigraphy. Figure courtesy Bill Hagopian, Johns Hopkins University.

Samples were collected from every lignite layer (denoted in black) except K', J', A', T, and U, and placed in Zip-lock plastic bags. Appearance of the samples ranged from dry, loose, light brown ashy material (e.g. H layer) to dark brown, moist, planar fragments (e.g. F' layer).

Wood samples from individual fossilized stumps were collected exclusively from the F layer and stored in glass jars. Associated paleosols were collected for several of the tree stumps and stored in glass jars and plastic bags. Resinite samples, consisting of grain-size to grape-sized nuggets, were collected *in situ* from fossilized tree stumps in the G', B' and M layers. One aggregate sample of resinite collected all over the site was labeled 'Mixed.' These were also stored in glass jars and plastic bags.

Shatterbox and Solvent Extraction

All samples that were not already fine-grained were pulverized in a Shatterbox for 1-2 minutes. The crushing chamber was cleaned in between each run with sand, soap and water, and three times each with methylene chloride and methanol.

The samples, no more than twelve grams each, were then packed into steel canisters for the Dionex Accelerated Solvent Extractor (ASE) 200. Each sample underwent organic extraction according to the following program:

Preheat: 0 minutes
Heat: 7 minutes
Static: 5 minutes
Flush: 100% volume
Purge: 60 seconds
Number of cycles: 3
Pressure: 1500 psi
Temperature: 150°C
Solvent: 50% methylene chloride in methanol

Because the samples were organic-rich, each sample was extracted twice.

A preliminary extraction had shown resinite extract to be too sticky for conventional ASE extraction. Therefore, each resinite sample was twice sonicated for six minutes in pure methanol, and then centrifuged five minutes at 3000 rpm to segregate the pellet of inextractable material from solvated organic matter.

Column Chromatography

The resulting total lipid extract (TLE) was separated using column chromatography in the following separation scheme (Figure 8).

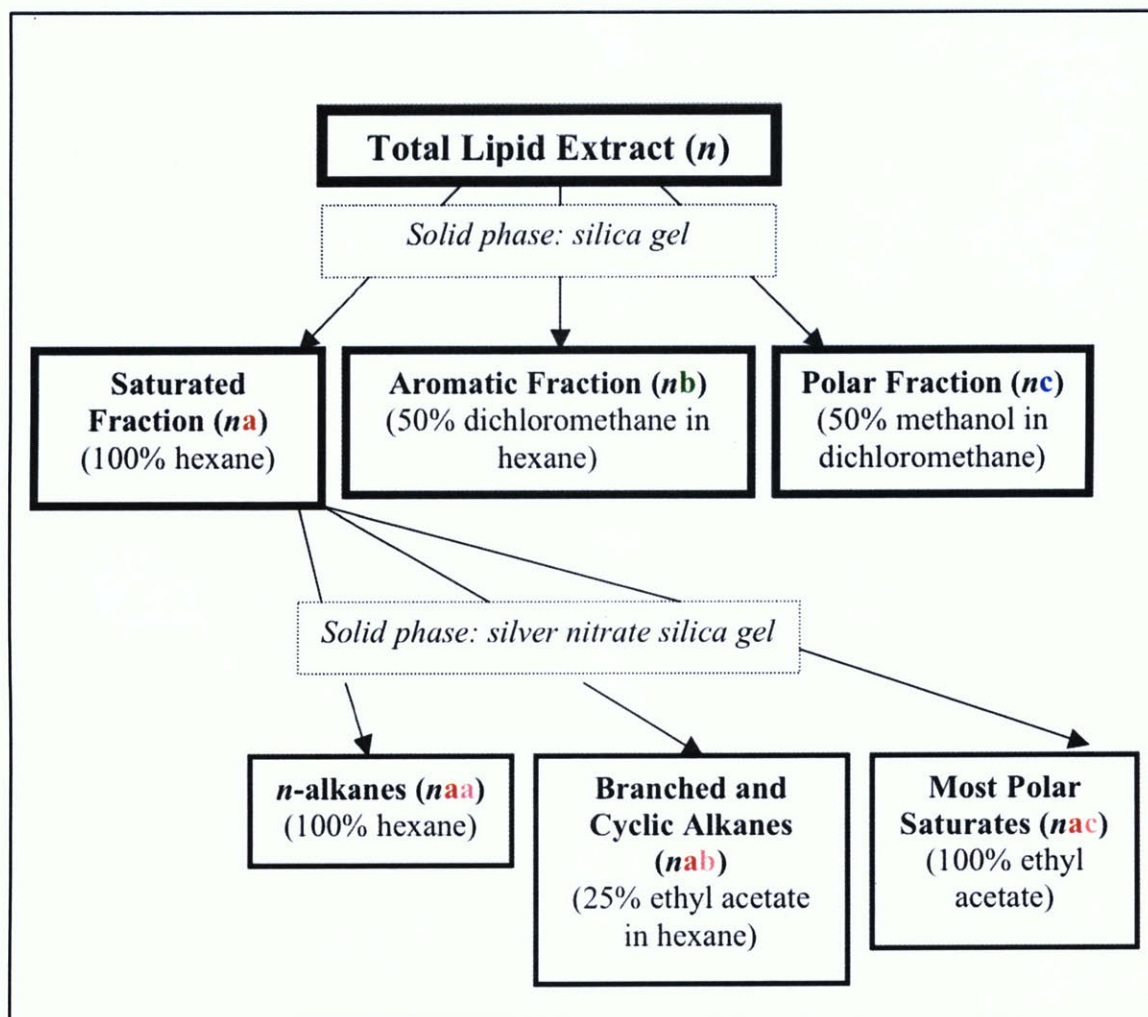


Figure 8. Separation scheme for biomarkers in Axel Heiberg TLEs of lignite, paleosol, wood and resinite samples.

Quantification

The saturated, aromatic and polar fractions (*na*, *nb*, *nc*) were quantified by weighing on a high-precision scale. All *naa* fractions, and selected *nab* and *nac* fractions, from the second separation were quantified for possible hydrocarbon biomarkers using a gas chromatograph flame ionization detector (GC-FID), an Agilent Technologies 6890N Network GC System.

. Each *naa* and *nab* fraction was concentrated in 50 μL hexane, from which an aliquot of 10 μL was withdrawn for analysis. The amount of material in each peak and each sample was calculated by the use of an external quantification standard, cholestane, or an internal quantification standard, aiC₂₂. Each sample series was run with a hexane blank. The oven temperature ramped according to either of two programs, a longer and a shorter one. Both were designed to ramp at the slowest rate over the elution range of the unknown peaks.

Z-LONG: total run time ~140 minutes				
	C/min	Next C	Hold (min)	Run time
1			80	0
2		4.5	320	0
3		4.5	320	0
4		10	325	28

Z-SHORT: run time ~67 minutes				
	C/min	Next C	Hold (min)	Run time
1			80	0
2		6	160	0
3		3	280	0
4		0		

GC-MS Analysis

Aliquots of sample were also analyzed on the Gas Chromatograph Mass Spectrometer, an Agilent 6890 with a Gerstel PTV (Programmable Temperature Vaporizing) inlet. These analyses were done to determine the structure of compounds being quantified (by GC-FID) and measured for isotopes (GCIRMS).

Structures were determined using AMDIS software (using the NIST library of mass spectra) or manually.

GCIRMS Analysis for Compound-Specific Hydrogen Isotopes

Of all *naa* and *nab* fractions analyzed, most (but not all) contained enough material to be analyzed by the lower-sensitivity ThermoFinnigan Delta Plus XP Continuous Flow Dual Inlet Isotope Ratio Mass Spectrometer. Each sample was analyzed at least in triplicate, or until material ran out. Aliquots were concentrated according to the amount of material needed to produce at least a 1000-millivolt signal given current instrument sensitivity. Therefore, aliquots ranged in volume from 50 μL (automatic injections) to 3 μL (manual injections). Each time, however, only 1 μL was injected for analysis.

Isotopic measurements for hydrogen are presented in standard deltaic notation, where SMOW = Standard Mean Ocean Water.

$$\delta\text{D} = 1000 \times [({}^2\text{H}/{}^1\text{H}_{\text{sample}})/({}^2\text{H}/{}^1\text{H}_{\text{SMOW}}) - 1] \quad (4)$$

The symbol ϵ denotes the isotopic effect associated with a certain process or pathway. That is,

$$\epsilon_{\text{product/reactant}} = \delta_{\text{product}} - \delta_{\text{reactant}} \quad (5)$$

Standards and Errors in Isotopic Measurements of δD

The 1 μL of sample was always coinjected with isotopic standards, with two, three or four peaks of known isotopic ratio that preceded or bracketed the sample peaks, including C_{11} , C_{16} , C_{20} FAME (fatty acid methyl ester), C_{36} , and/or C_{40} . All isotopic standards were prepared and supplied by Dr. Arndt Schimmelman of Indiana University. C_{16} was most frequently used. Within a given sequence, the same standard peaks were used for consistency. The sample peaks' isotope ratios were then calibrated to these standard peaks.

The instrument's performance was evaluated on a daily basis, using standard mixtures of peaks with known isotopic ratios. These standards, Arndt A and Arndt B⁴, are both composed of the *n*-alkanes of chain length C_{16} through C_{30} , differing only in relative concentrations of those peaks.

Two measurements are used to evaluate the instrument's precision and accuracy on a given day: RMS, and the H3+ factor.

1) RMS is derived from the degree to which Arndt A and/or Arndt B measured isotope values deviate from the known isotope values on a given day. The RMS deviation incorporates both accuracy and precision, and is therefore the most useful and conservative benchmark for these analyses. A sample calculation is given in Table 2.

⁴ Courtesy Arndt Schimmelman, University of Indiana, Bloomington.

Peak	Actual	Measured	Difference
C ₁₆	-73.9	-73.9	0
C ₁₇	-142	-145.751	-3.751
C ₁₈	-55.2	-54.551	0.649
C ₁₉	-119.4	-122.612	-3.212
C ₂₀	-48.7	-48.257	0.443
C ₂₁	-215	-217.446	-2.446
C ₂₂	-62.2	-62.881	-0.681
C ₂₃	-46.5	-47.255	-0.755
C ₂₄	-55.4	-53.539	1.861
C ₂₅	-256.4	-258.952	-2.552
C ₂₆	-57.7	-60.072	-2.372
C ₂₇	-226.5	-229.901	-3.401
C ₂₈	-52.4	-52.268	0.132
C ₂₉	-182.1	-178.345	3.755
C ₃₀	-42.7	-42.7	0
SUM(diff^2)			73.307756
RMS			8.561994861

Table 2. Sample calculation for daily RMS based on Arndt standards, composed of peaks with known D/H isotopic composition, which is shown in the column “Actual.” “Measured” is the measured value on a given day, and the next column gives the difference. Below are two numbers: the SUM of each difference squared, and the square root of SUM, which is the RMS error.

2) The H3+ factor is a measure of how much tritium is being created in the reactor, along with deuterium. Since the instrument reads tritium as deuterium, a correction is applied to reduce the measured deuterium by the tritium factor, i.e., the H3+ factor. The H3+ factor is calculated over a range of amplitudes (i.e. a range of gas pressures) that ideally bracket the range of amplitudes of unknown sample peaks. The software then incorporates this factor into reported δD values. The more important parameter, then, is not the H3+ correction itself, but rather the degree of variance of H3+ factor over the range of peak amplitudes.

RMS and H3+ measurements for the duration of analysis are given in Table 3.

Date	RMS	H3+ factor	H3 Stdev
6/9/04		5.68	2.65
6/23/04		5.28	1.78
6/25/04		8.36	1.64
6/28/04		5.68	2.55
12/10/04		3.89	3.5
12/12/04	6.56	4.14	5.45
12/13/04		4.07	4.66
12/14/04		3.9	1.54
12/15/04	5.12	4.48	7.09
12/16/04	13.04	9.99	15.91
12/17/04	11.66	4.21	5.46
12/18/04	9.02	3.91	1.55
12/19/04	8.87	4.12	4.17
12/20/04		4.27	5.15
1/3/05	5.12	4.26	4.95
1/4/05	5.85		
1/8/05	5.22	3.97	3.38
1/9/05	7.26	3.85	1.3
1/10/05	4.22	4.22	5.76
1/11/05	5.04	3.85	1.33
1/12/05	4.83	4.3	1.45
1/28/05	7.11	4.27	2.91
2/10/05	4.46	3.84	4.73
2/13/05	3.16	3.88	2.74
average	6.66	4.71	3.98
standard dev.	2.75		3.11

Table 3. Summary of daily RMS, H3+ factor and standard deviation of H3+ factor over the duration of analyses. For days where data are missing, either the data were unavailable, the peaks were too small to be reliable (RMS) or the software crashed (H3+ factor).

The H3+ factor is applied to the data by the software, so there is no need to re-apply it to the reported values. However, the variation in H3+ measurements over the range of gas pressures should be taken into account.

Error thus far, therefore, must compile RMS and H3+ factor variance. In addition, a third error must be applied: a calibration error. Ideally, the range of unknown peaks should be calibrated by four peaks from the coinjection standard: one “throwaway” peak

of low molecular weight⁵, two peaks bracketing the range of unknown peaks, and one peak to calibrate the other two.

However, this could not always be accomplished, due to two factors: 1) standard peaks coeluting with the unknown peaks on either side; and 2) standards of high molecular weight (e.g. C40) coming out of solution and yielding broad, unreliable peaks. In these cases, only two standard peaks were included in the coinjection standard: C₁₁ and C₁₆, acting as a throwaway peak and a single calibration peak, respectively.

Calibrating to only one standard, on only one side of the data, is a non-ideal situation. Therefore, we compiled data from several chromatograms where both C₁₆ and C₃₆ were present as standards. The offset between calibrating to one standard (C₁₆) and to both (C₁₆ and C₃₆) is as follows:

⁵ The “throwaway” peak is necessary because the first compound to elute will never be read correctly by the GCIRMS, likely due to memory or conditioning effects. Schimmelman: <http://php.indiana.edu/~aschimme/hc.html>.

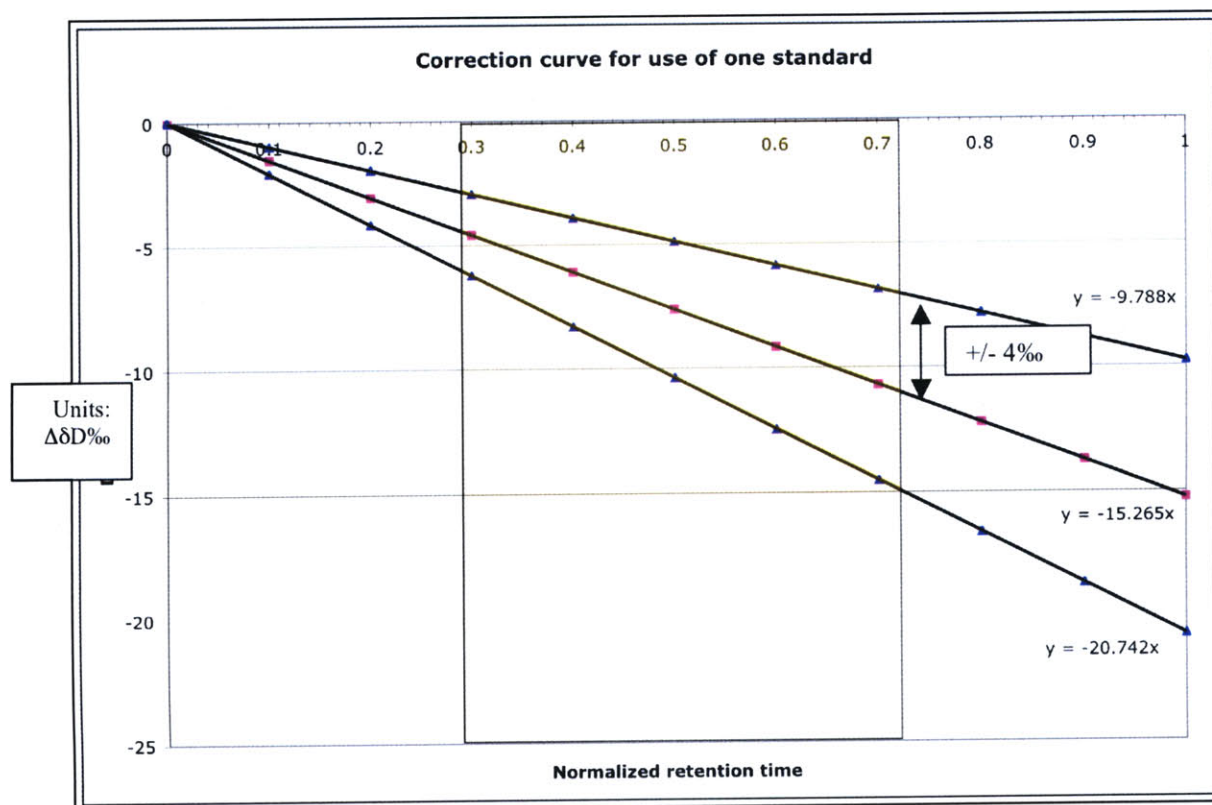


Figure 9. Correction curve for peaks in chromatograms with only one standard peak, C_{16} . The middle curve (pink points) represents the average slope compiled from nine linear relationships, from nine samples that contained both C_{16} and C_{36} standard; the outside curves (blue points) represent the standard deviation of that slope. Y-intercept was very close to zero, as expected. Unknown peaks were first calibrated only to C_{16} , then to both C_{16} and C_{36} to determine the difference in calibrated values. The difference increases linearly with increasing distance away from C_{16} and towards C_{36} . (The distance is normalized; that is, every distance between C_{16} and C_{36} is treated = 1.) Therefore, peaks farther away from C_{16} will need a larger correction with a larger error attached. The orange box indicates the span that includes C_{23} - C_{29} .

This correction can thus be applied to peaks where C_{16} was the only standard peak available. Note that y-intercept values were very close to zero, as expected. Note also that the farther from C_{16} peaks are, the greater correction they will need, and with a greater attached error. Our peaks of interest – C_{23} through C_{29} odd – fall within a finite range of 0.29 to 0.72 normalized retention time (NRT). The greatest error that ever need be

applied, then, is $\sim 4\text{‰}$ to values for C_{29} . (4‰ is the difference between the average correction line in pink, and the maximum and minimum correction lines in blue, at $NRT=0.72$, where C_{29} elutes.)

$$\text{Corrected } \delta D = -15.265 \text{ (Original } \delta D) \pm 4\text{‰} \quad (6)$$

We now have three sources of error: RMS, $H3+$ factor variation, and calibration error. One final error remains: the precision among multiple measurements. Samples were measured in triplicate whenever possible. In many cases, where manual injections were necessary because of low abundance, material ran out after two trials, and the third trial yielded peaks too low to have a trustworthy isotopic value. When that occurred, the standard deviation is reported from only two values, because the third is an obvious outlier.

The mean standard deviation for multiple measurements was $1.99 \pm 1.55\text{‰}$. The largest error was 6.19‰ (for C_{29} in the G layer), and the next largest was 4.83‰ . In several cases, a sample may have been run in triplicate or duplicate repeatedly, with weeks or months having passed between runs. In those cases, the most robust data set was reported. “Robustness” was evaluated according to the errors described, wherein the data set with the least error was chosen.

Three sources of error, therefore, must be considered in every measurement; four sources of error must be considered in the cases where the data were calibrated only to C_{16} (about a third of all data). In sum, the total uncertainty of each data point is $\sim 12.5\text{--}16.5\text{‰}$, which is roughly equivalent to 1‰ uncertainty for oxygen isotopes.

Summary of errors for δD measurements	
RMS (precision and accuracy of instrument)	6.66 +/- 2.75‰
H3+ factor variation (precision of H3+ factor over a range of gas pressures)	3.98 +/- 3.11‰
Calibration error (due to calibration to only one peak)	depends on normalized retention time relative to C ₁₆ maximum 4‰
Precision of unknown peaks due to multiple measurements	variable (indicated as error bars on graphs) average 1.99 +/- 1.55‰

Table 4. Summary of errors for δD measurements in this study.

Elemental Analysis for Bulk Carbon Isotopes

Original, unextracted lignite material from each sample was analyzed for bulk carbon isotopes. Aliquots of 0.200 μg to 1.100 μg were wrapped in aluminum foil for the autosampler. Each sample was analyzed in triplicate. In between each triplicate run, a blank and a standard of known isotopic composition (PSU kerogen, NBS-22 oil, or IAEA-6 sucrose) were also run. These standards were used to estimate the precision and accuracy of the instrument on a given day. In every case, the deviation from accepted values was so small that correction to values for unknowns was unnecessary.

Isotopic measurements for carbon are presented in the same standard deltaic notation described for hydrogen, except the standard is Pee Dee Belemnite (PDB).

$$\delta^{13}\text{C} = 1000 \times [({}^{13}\text{C}/{}^{12}\text{C}_{\text{sample}})/({}^{13}\text{C}/{}^{12}\text{C}_{\text{VPDB}}) - 1] \quad (7)$$

IV. Results and Discussion

The results described in this section will be used to address the possible magnitude, frequency and cause(s) of Middle Eocene climate variability on Axel Heiberg Island. The different proxies will be used to illuminate different parameters.

- 1) Biomarker structures, i.e. acetogenic vs. isoprenoid, highlight what kind of source organisms existed, and what metabolic pathways were at work.
- 2) The absolute abundances of *n*-alkanes may indicate the intensity of floristic input, either by floristic abundance or increased preservation. The relative abundances of *n*-alkanes indicate what types of plants dominated the ambient ecosystem.
- 3) Hydrogen isotopic ratios of specific compounds give information about the isotopic ratios and provenance of source water.
- 4) Bulk carbon isotopic ratios in lignites may indicate $\delta^{13}\text{C}_{\text{atmosphere}}$.

Preliminary Data

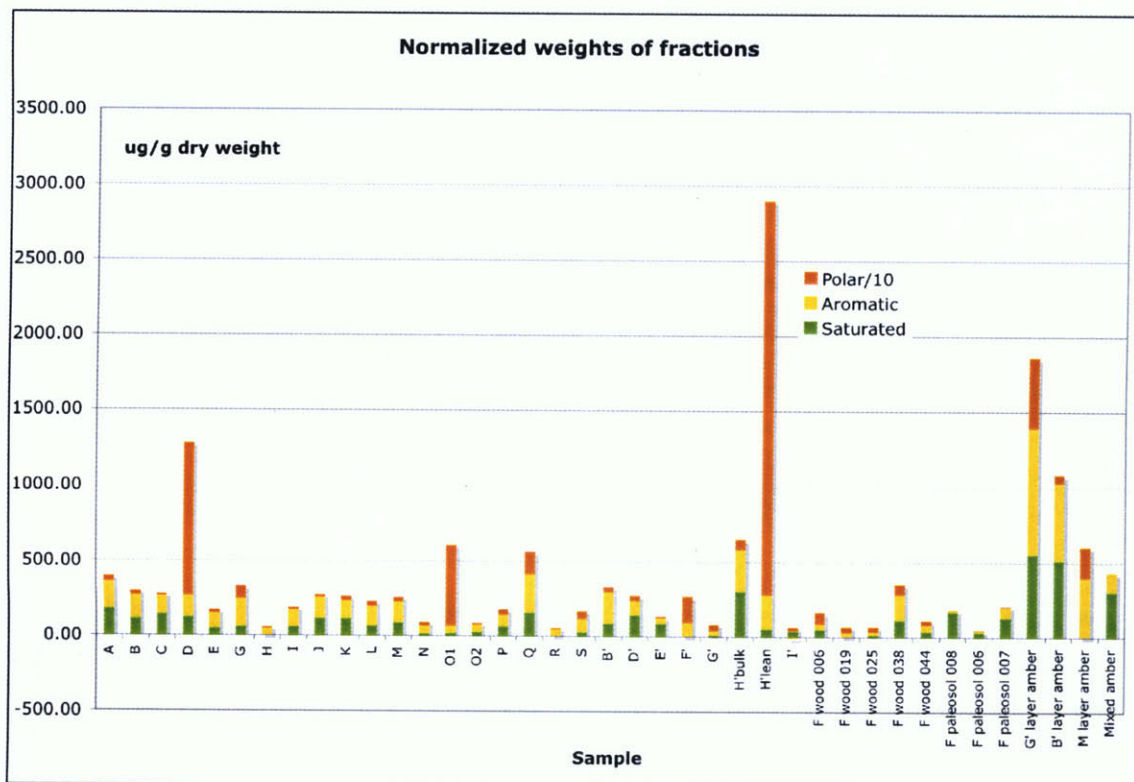


Figure 10. Breakdown of saturated, aromatic and polar fractions (normalized against dry weight) from each sample's total lipid extract (TLE). Note: Polar fraction weight is divided by ten for purposes of scale. Saturated fractions were collected with hexane solvent. Aromatic fractions were collected with 1 : 1 hexane : DCM. Polar fractions were collected with 1 : 1 DCM : methanol. Letters (A through I) denote lignite/lignite layers. 'F wood' denotes individual tree stumps from the F layer. 'F paleosol' denotes the paleosols associated with selected individual tree stumps. Resinite samples, at far right, were collected *in situ* from tree stumps, except for 'Mixed resinite,' which was collected from various layers.

After ASE extraction, the total lipid extract (TLE) was separated by column chromatography into saturated, aromatic and polar fractions. The normalized weight of each fraction in each sample is shown in Figure 10. (Note: the polar fraction is reduced by one order of magnitude for the purpose of scale.)

As expected, lignites and resinite have the most extractable organic material per gram dry weight, averaging 2126 $\mu\text{g/g}$ and 2662 $\mu\text{g/g}$, respectively, though with considerable variation. The wood samples have far less extractable material at an average value of 619 $\mu\text{g/g}$, and paleosols the least, with 199 $\mu\text{g/g}$. Wood is made up of tough polymers such as lignin and cellulose, so it is not surprising that little material was extracted (Campbell 1999). Paleosols are made up of mostly carbonate calcareous matrix (Ekart 1999), which explains the low value of extractable organic matter.

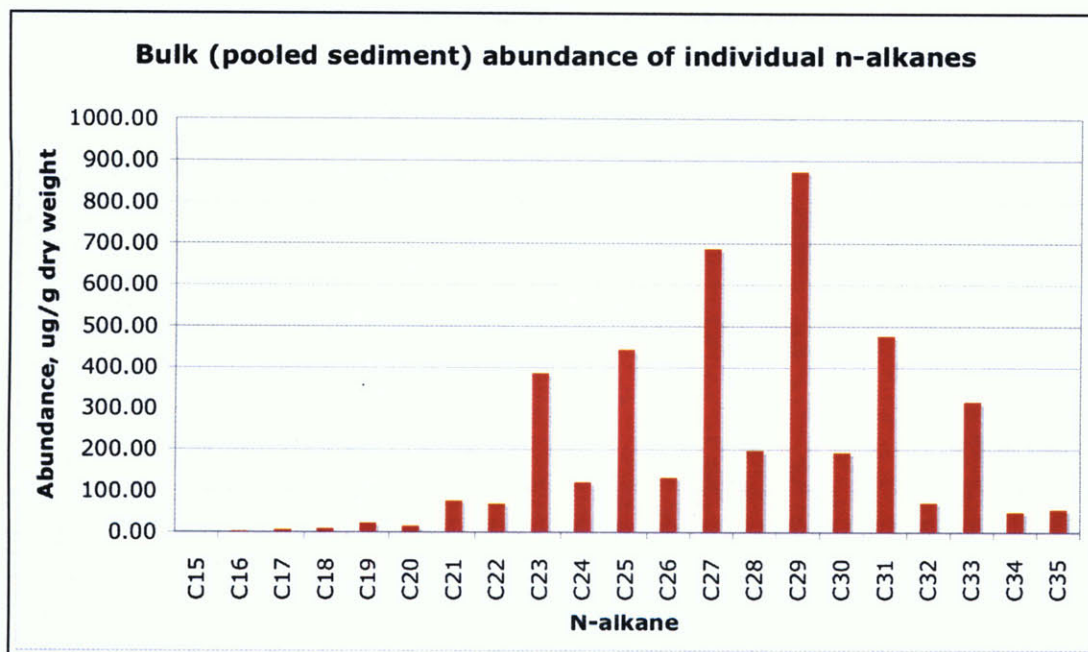


Figure 11. Pooled, normalized abundances of individual *n*-alkanes over all lignite layers. Data were obtained using GC-FID quantification with an internal or external standard, and GC-MS identification.

Figure 11 shows the overall abundance of *n*-alkanes in the Axel Heiberg lignite layers. This odd-over-even predominance is characteristic of fossil flora: the fatty acids from which *n*-alkanes are derived are built two carbons at a time, but during diagenesis,

decarboxylation occurs, resulting in a chain with one less carbon (Staccioli 2002). C_{29} predominates. This is in accordance with the finding of Yang (2004), who found that C_{29} predominance is characteristic of a whole-leaf signature instead of leaf surfaces alone, which have C_{25} predominating. C_{29} is followed by C_{27} , C_{31} , C_{25} , C_{23} and C_{33} by abundance. Though this pattern was most often observed in each lignite layer, for some samples the distribution's maxima shifted to slightly shorter or longer-chain *n*-alkanes.

Based on the data in Figure 12, we can further speculate on the chemical configuration of the *n*-alkanes' precursors. They could have been any of *n*-alkanes, secondary alcohols, ketones, fatty alcohols, fatty acids, aldehydes or wax esters. Wax esters are made by conjoining fatty alcohols and fatty acids, so their chain length is approximately double that of the separate components (Kunst 2003). However, during diagenesis, the ester group is susceptible to breakage.

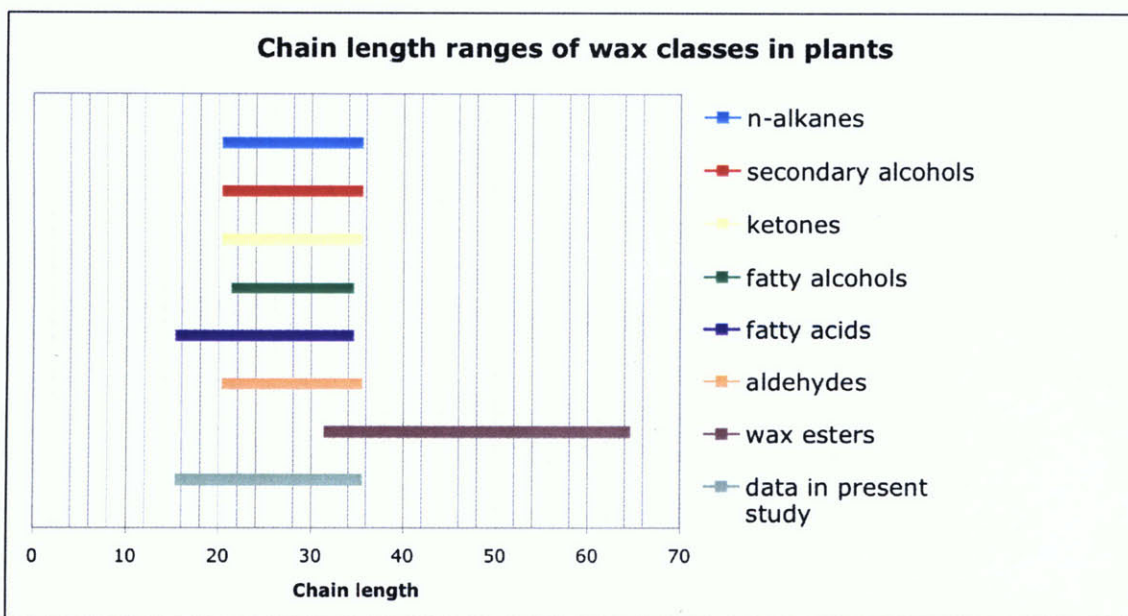


Figure 12. The ranges of chain lengths particular to wax classes in plants, compared to data in present study. Data from Kunst 2003.

There are three pathways by which plants synthesize wax hydrocarbons. The acyl reduction pathway produces wax esters and primary alcohols. However, the majority of wax hydrocarbons are synthesized in epidermal cells via the decarbonylation pathway (Millar 1999). C_{18} moieties are produced by *de novo* fatty acid synthesis in the plastid, and their isotopic composition is derived half from NADPH and half from the acetate precursor (see Figure 5; Hayes 2001).

Aldehydes directly precede the formation of alkanes, secondary alcohols, and ketones. (This explains the similarity of chain length ranges in Figure 12.) However, aldehydes undergo decarbonylation – the loss of one carbon – to produce odd-chain hydrocarbons. Given that there are comparatively very few n-alkanes with a chain length $< C_{18}$ found in this study, we may conclude that the majority came from the decarbonylation pathway, and that the predominantly odd chain lengths were a natural consequence of this pathway rather than an artifact of diagenesis.

The lipids' various functional groups are of interest to this study because of reductions that may have occurred during diagenesis. Specifically, we would expect the aldehydes, secondary alcohols, and ketones to have acquired an additional hydrogen from ambient environmental water. However, this newly introduced hydrogen would comprise only 1-2% of the hydrogen isotope signal, introducing a negligible error.

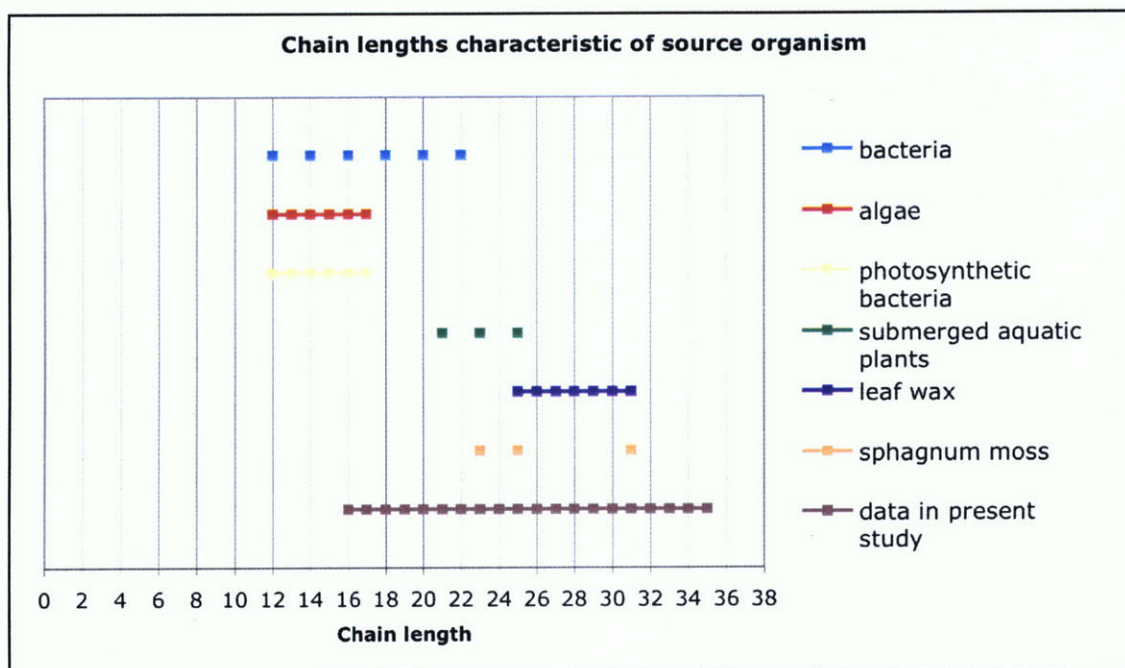


Figure 13. *N*-alkane chain lengths characteristic of the source organism, compared to data from present study. Data compiled in Sachse (2004).

Having discussed the pathway involved in making the *n*-alkanes, we turn to the classes of organisms that may have synthesized them (Figure 13, data compiled in Sachse 2004). The values listed for submerged aquatic plants are derived from a study of four modern lacustrine environments on Mount Kenya in East Africa (Ficken 2000).

Sphagnum is a taxon of moss common to peat deposits (Baas 2000) and indicative of wet soil (Upchurch 1998).

If the ranges and distributions of *n*-alkanes in Figure 13 are compared with those in the lignite layers (Figure 11), it is clear that bacteria, algae and photosynthetic bacteria contributed very little, if anything, to the lignite deposits. Rather, the *n*-alkanes come from submerged aquatic plants and higher plant leaf wax. *Sphagnum* moss can be

discounted because, despite its presence in some Eocene pollen assemblages (Upchurch 1998), it was not found on Axel Heiberg Island (McIntyre 1991).

This assertion, that the *n*-alkanes come from higher plants and submerged aquatic plants, is consistent with the existing evidence of the Axel Heiberg forest. The forest was part swamp, and grew on a floodplain adjacent to an evolving orogeny (Ricketts 1991). The layers were buried in massive flood events (Yang 2004).

The paucity or absence of short-chain *n*-alkanes is also telling, since bacteria make *n*-alkanes with chain lengths of 12-22 (Sachse 2004). Also, bacteria rework longer-chain *n*-alkanes from higher terrestrial input, resulting in short-chain *n*-alkanes. This may reflect a limited bacterial presence, or more likely, an overwhelming plant presence that dominates the bacterial signal.

Bulk Carbon Isotopes

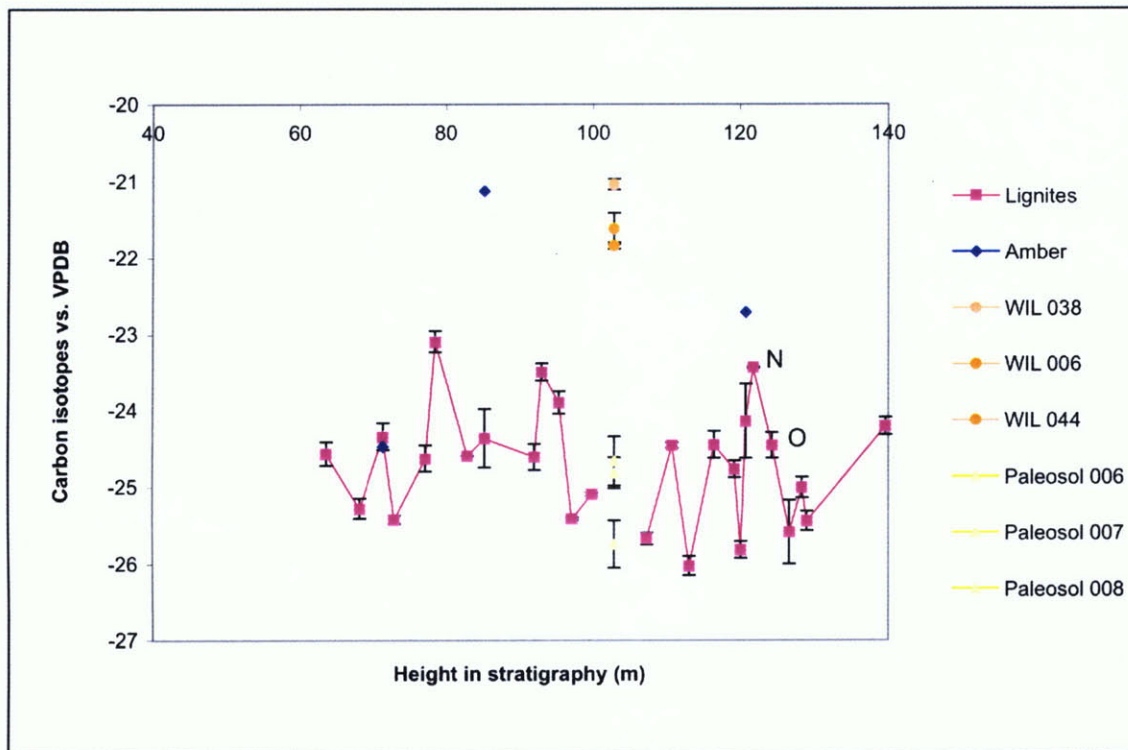


Figure 14. Measurements of bulk carbon over the whole lignite layer stratigraphy, as well as values from F layer fossilized wood stumps (denoted “WIL”), associated paleosols, and embedded resinite.

Figure 14 shows bulk carbon isotope measurements for all samples, including lignites, wood, resinite and paleosols. (Note that the lignite layers are rarely physically adjacent, but are usually sandwiched between siltstone, sandstone or clay layers.) Several features are notable.

1) First, in adjacent lignite layers, bulk carbon isotopes differ by an average of 1.0 +/- 0.6‰. From the O to the N layer (from 124.3 m to ~121.8 m, respectively), there is a jump of ~1‰ to heavier isotopes. Richter (2005) sampled the siltstone interposed

between these two layers. The pollen assemblages indicated that the level O forest had been buried in a catastrophic flood, and replaced by a broad-leaved deciduous forest. Studies of modern trees indicate that in fact, broad-leaved deciduous trees are *lighter* than conifers: $-27.2 \pm 1.5\%$ vs. $-26.0 \pm 2.1\%$ (data compiled in Flanagan 1997). While these values may not be statistically different, we will still discuss the possible causes of the difference. It may have to do with the fact that broad-leaved deciduous stands are denser, and therefore more subject to the “canopy effect,” whereby light carbon from the forest floor is recycled within the ecosystem (Broadmeadow and Griffiths 1993).

Another option is the difference between conifers’ and broad-leaved species’ rates of carbon assimilation. Previous studies have shown that conifers, or boreal species, have lower photosynthetic capability. In some cases, it is enough to explain this effect by cold, nutrient-poor northern soils and a short growing season (Flanagan 1997). However, these conditions did not exist on the Eocene Axel Heiberg Island.

In other studies, lower CO₂ assimilation was attributed to leaf morphology: conifers have longer, narrower leaves with lower stomatal conductance. Therefore, their stomata retain more water and assimilate less carbon. This effect, along with the fact that conifer forests are more open and therefore more resistant to the canopy effect, has been used to explain carbon isotope discrepancies between conifer and broad-leaved/angiosperm flora (Murray 1998). Conifer wood is also generally heavier than angiosperm wood (e.g. Stuiver and Braziunas 1987).

However, contrary to these trends, our data show a jump to *heavier* values coincident with establishment of the broad-leaved forest. A number of factors may be responsible for this discrepancy. The broad-leaved vs. conifer studies were based on the

carbon isotopes of leaves exposed to the sun (Flanagan 1997), while the lignites in this study are assumed to represent the integrated abscission of all leaves. However, given that modern *Metasequoia* prefer growing on open soil, do not tolerate shade and grow in a conical shape that maximizes sun exposure, most of the fossil leaves were probably exposed to sunlight.

If the *Metasequoia* was not unusually depleted, the succeeding broad-leaved deciduous flora may have been unusually enriched. Without knowing more about the specific taxa present, we can only assume that this enrichment would have been due to a change in $\delta^{13}\text{C}_{\text{atmosphere}}$.

Another possibility is that the broad-leaved deciduous stand that succeeded the deciduous conifer stand was relatively open. That is, it was not subject to the depletive canopy effect that characterizes densely-packed broad-leaved forest stands (Broadmeadow and Griffiths 1993).

One final possibility is that the values reported in Flanagan (1997), $-27.2 \pm 1.5\text{‰}$ vs. $-26.0 \pm 2.1\text{‰}$, are not statistically different, so the isotopic jump cannot be attributed to a change from boreal to broad-leaved stands.

Two more factors may contribute to the lignites' $\delta^{13}\text{C}$ signal. First, trees distal to the watercourses would have contributed more to sediments, because the material shed by trees proximal to the watercourses would have washed downstream. Trees distal to the watercourse, however, are not necessarily distal to the stand, and therefore no further conclusions can be made from this consideration. Second, $\delta^{13}\text{C}$ values might have been

increased by the salinity flux that accompanies slow flood events (Farquhar 1989). This salinity increase would explain the $\delta^{13}\text{C}$ jump from the O to N layers.

2) Second, the isotopes never follow a unidirectional trend for more than three layers. Rather, the isotopes vacillate from lighter to heavier and back again in successive layers. First-order interpretation of these data suggests highly variable $\delta^{13}\text{C}_{\text{atmosphere}}$, given that $\delta^{13}\text{C}_{\text{atmosphere}}$ is the primary control on $\delta^{13}\text{C}_{\text{plant}}$ (Arens 2000).

3) Third, though there are limited data, there seems to be a marked difference in the isotopic signatures between 1) lignite and resinite and 2) lignite and wood. Resinite and wood are both generally heavier than the lignite. This is consistent with previous studies, which have shown that cellulose (both in wood and leaves) is isotopically heavier than lipids (Schoell 1984, Leavitt and Long 1982).

However, the resinite data set consists of only three points, and the offset from the lignite value is not consistent (0.13‰, 3.2‰, and 1.4‰ from left to right). Resinites (interchangeable with resinite) are polymers made up of labdanoid diterpenes, i.e. C_{20} isoprenoids, which are made by the MEP pathway in the chloroplast. This pathway produces lipids far more depleted in ^{13}C than their C_{15} and C_{30} MVA counterparts, and also relative to bulk leaves (Chikaraishi 2004b). Thus, we would expect resinites to be *lighter* than the leaves, not heavier. There are two possible explanations for this discrepancy: either the leaves contain more C_{20} isoprenoids by concentration, or the lignite layers represent an integrated value that does not correspond with the resinite

samples, which were taken directly from fossil tree stumps, and represent far shorter, more discrete periods of time.

Smith (1982) reported bulk resinite $\delta^{13}\text{C} = -24.7\text{‰}$ for Australian coals. The mean resinite $\delta^{13}\text{C}$ in all literature is $-22.8 \pm 1.7\text{‰}$ (Murray 1998 and references therein). Our data place resinite $\delta^{13}\text{C}$ at $-24.5 \pm 0.29\text{‰}$ (G' layer), $-21.1 \pm 0.16\text{‰}$ (B' layer), and $-22.7 \pm 0.19\text{‰}$ (M layer). Taken together, our resinite $\delta^{13}\text{C}$ values average $-22.8 \pm 1.7\text{‰}$, exactly matching the average and standard deviation of previously reported values. These previous values were taken from resinites originating in Israel to Canada to New Zealand, from the early Cretaceous to the late Holocene (though this data point is a temporal outlier), mostly centering on the Tertiary. The consistency of values may indicate uniformity of atmospheric $\delta^{13}\text{C}$ during the time the samples represent, or it may be a coincidence.

Modern resins are lighter than ancient resinites, at $-25.8 \pm 1.5\text{‰}$. This may be because industrial activity (with the burning of fossil fuels) has depleted atmospheric carbon enough to deplete plant matter by that magnitude, or that the conditions conducive to resinite preservation are coincident with ^{13}C enrichment (Murray 1998). As mentioned before, this may include disproportionate contributions by distal trees (Farquhar 1989).

The wood data set is also limited, being confined to one layer, and without a complementary lignite value. However, the values cluster around a relatively heavy value ($-21.66 \pm 0.45\text{‰}$). This is surprising, given that modern cellulose and lignin usually register approximately -28.5‰ and -29.5‰ , respectively (Grocke 2002). However, when plant components are compared relative to each other, wood and leaf cellulose are always heavier than lignin, which is in turn heavier than lipids (Murray 1998). The modern

cellulose may be depleted relative to ancient cellulose for the same reasons that modern resin is depleted relative to ancient resin: the industrial burning of fossil fuels has depleted atmospheric carbon with regard to ^{13}C .

According to the equation put forth by Farquhar (1989) and modified by Arens (2000), $\delta^{13}\text{C}_{\text{atmosphere}}$ can be estimated using $\delta^{13}\text{C}_{\text{plant}}$.

$$\delta^{13}\text{C}_{\text{CO}_2} \text{‰} = (\delta^{13}\text{C}_{\text{plant}} \text{‰} + 18.67) / 1.10 \quad (8)$$

Using this equation, $\delta^{13}\text{C}_{\text{atmosphere}}$ was plotted against the stratigraphy (Figure 15).

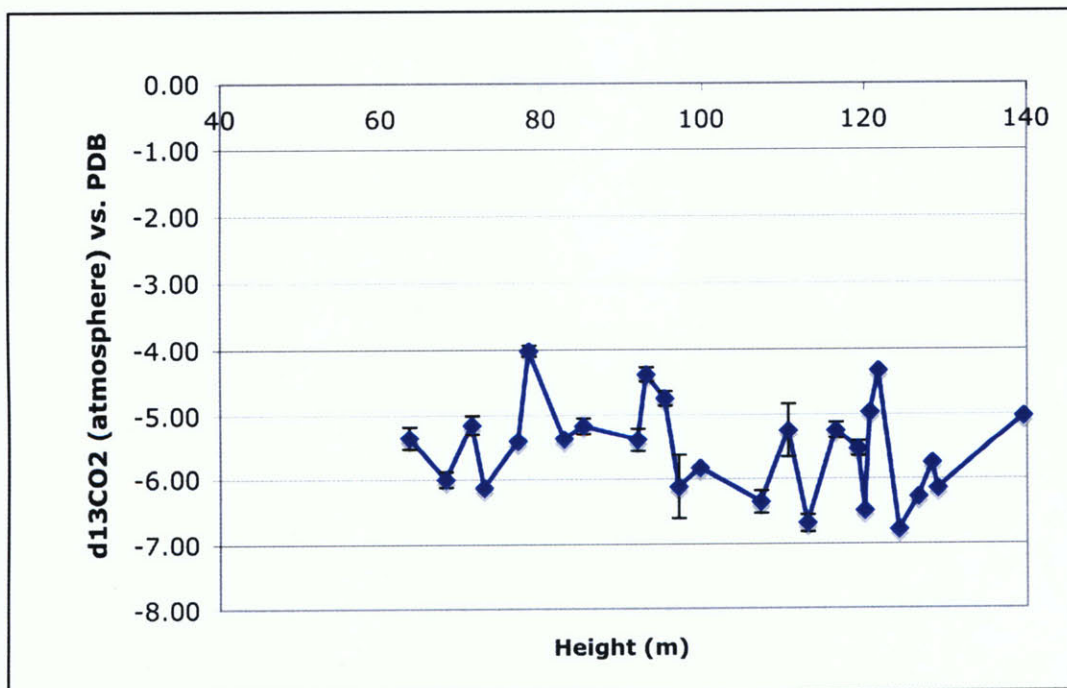


Figure 15. $\delta^{13}\text{C}_{\text{atmosphere}}$ across the Axel Heiberg stratigraphy, as calculated by Equation (8) (Arens 2000). Values of bulk lignite were used for $\delta^{13}\text{C}_{\text{plant}}$.

In succeeding layers, $\delta^{13}\text{C}_{\text{atmosphere}}$ may change by nearly 3‰, as seen in the O → N transition described previously. Enormous pulses of methane on time scales as short as decadal have been observed for interstadial time periods (Kennett 2000). If the data are accurate, pulses of light carbon flooded the Arctic atmosphere; the question is, over how long? These data are not known, as ash layers are absent in the Axel Heiberg stratigraphy, which precludes radiometric dating.

Retallack (2001, 2002) summarized atmospheric pCO_2 over the past 67 Ma by stomatal indices of fossil *Ginkgo*. One data point exists for the Early Eocene (2000 ppmv CO_2), and none for the Middle Eocene. In the latest Eocene, the atmospheric concentration of CO_2 drops to ~1700 ppmv. Pearson and Palmer (2000) estimated 2000 ppmv by boron isotopes in calcite shells. Ekart (1999) estimated 900 ppmv from paleosol paleobarometers. Royer (2001) estimated 320 ppmv by studying stomatal indices, the same method as Retallack (2002). Berner and Kothavala (2001) estimated 700 ppmv from the GEOCARB II carbon cycling model. Yapp (2004) estimated 2700 +/- 300 ppmv from pedogenic goethite. Clearly, different proxies lead to very different estimates of pCO_2 .

pCO_2 and $\delta^{13}\text{C}_{\text{atmosphere}}$ are not necessarily correlated unless the sources of carbon are constrained. Therefore, it is difficult to attempt estimating pCO_2 with our estimates of $\delta^{13}\text{C}_{\text{atmosphere}}$.

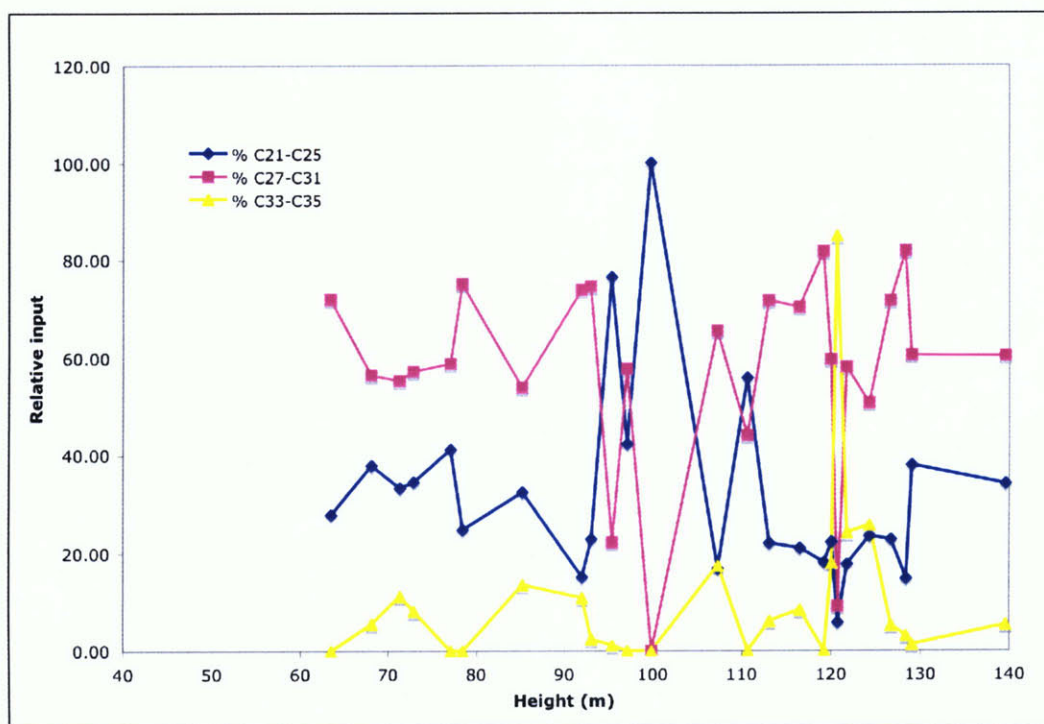


Figure 16. Relative inputs of *n*-alkane chain length groups, odd-numbered only. C₂₁-C₂₅ represent submerged aquatic plants; C₂₇-C₃₁ represent higher plant waxes; C₃₃-C₃₅ represent higher plant waxes and another possible source, made distinct by the dramatic peak in the M layer (~120 m).

4) Fourth, as can be seen in Figure 16 in comparison with Figure 14, the relative inputs of *n*-alkane chain length groups is unrelated to bulk carbon measurements. Figure 16 shows that, though higher plant input (C₂₇-C₃₁) is the norm, occasionally the other groups (C₂₁-C₂₅ for submerged aquatic plants and C₃₃-C₃₅ for higher plant waxes and/or an additional unknown contributor) dominate. The aberrations in this record do not correlate significantly with aberrations in the bulk carbon isotope record (Figure 11); the signals are unrelated ($R^2=0.002$). However, the signals recorded in bulk organic carbon are almost certainly not from flora alone. Without compound-specific carbon data, we cannot conclude that the fluctuations in carbon isotopes are attributable to environmental, rather than floral, fluctuations.

In this record, there are two notable deviations from the norm. One occurs in the M layer, around 120m, where the C₃₃-C₃₅ signal spikes. Here, the bulk $\delta^{13}\text{C}$ signal also reaches a local maximum, that is, a heavy value that deviates significantly from the previous data point. The M layer lignite was markedly rich, almost black in color. It could be that $\delta^{13}\text{C}_{\text{atmosphere}}$ became heavier at this time, and the increase in chain length was an unrelated floristic change. On the other hand, it could be that the increase in chain length was due to warmer temperatures, to prevent excess evapotranspiration, or serve as a more robust barrier against rain droplets or parasites.

The other deviation occurs in the E layer, around 100m, where the signal attributed to submerged aquatic plants spikes. The E layer lignite was colored markedly light, a fine, medium brown, ashy soil. There are no significant maxima or minima in $\delta^{13}\text{C}$ that coincide with this deviation. This layer could represent a shift to more swamp-like conditions after a flood event, before a forest reestablished itself.

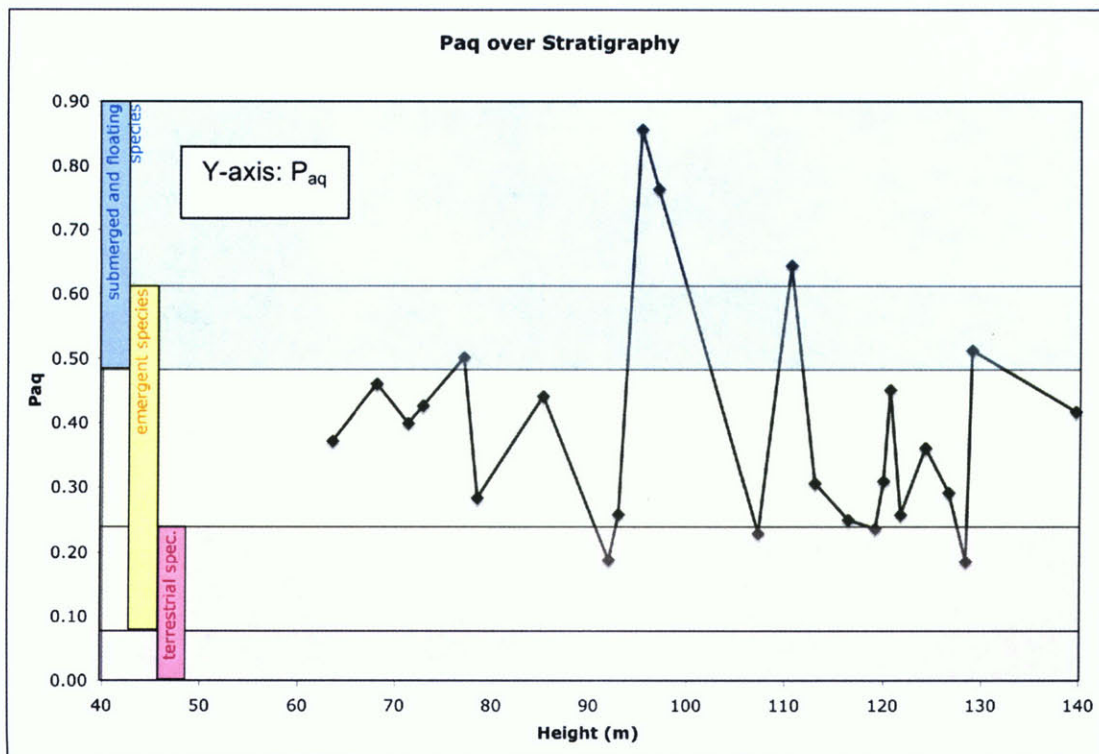


Figure 17. P_{aq} (a proxy for input of submerged aquatic plants) for the Axel Heiberg stratigraphy, calculated according to Equation (9) (Ficken *et al* 2000). For modern plants, $P_{aq} < 0.25$ indicates terrestrial input; $0.1 < P_{aq} < 0.4$ indicates emergent macrophytes; $0.4 < P_{aq} < 1.0$ indicates submerged or floating macrophytes. For ancient deposits, P_{aq} may indicate a mixture of the three inputs.

Ficken *et al.* (2000) developed an *n*-alkane proxy for input of submerged aquatic plants, termed P_{aq} , shown in Equation (9) and Figure 17.

$$P_{aq} = (C_{23} + C_{25}) / (C_{23} + C_{25} + C_{29} + C_{31}) \quad (9)$$

For modern plants, $P_{aq} < 0.25$ indicates terrestrial input; $0.1 < P_{aq} < 0.4$ indicates emergent macrophytes; $0.4 < P_{aq} < 1.0$ indicates submerged or floating macrophytes. However, for ancient sediments, the P_{aq} value may represent a mixture of more than one input. Given the microfossil assemblages and the prevalence of higher wax *n*-alkane

chains, this is probably the case for the majority of points that fall within the range of “emergent species.” At the E layer, consistent with the other data, there is a spike towards submerged plant input. At the M layer, there is a dip towards pure terrestrial input. Again, there is no correlation with the bulk carbon isotope record ($R^2=0.00091$).

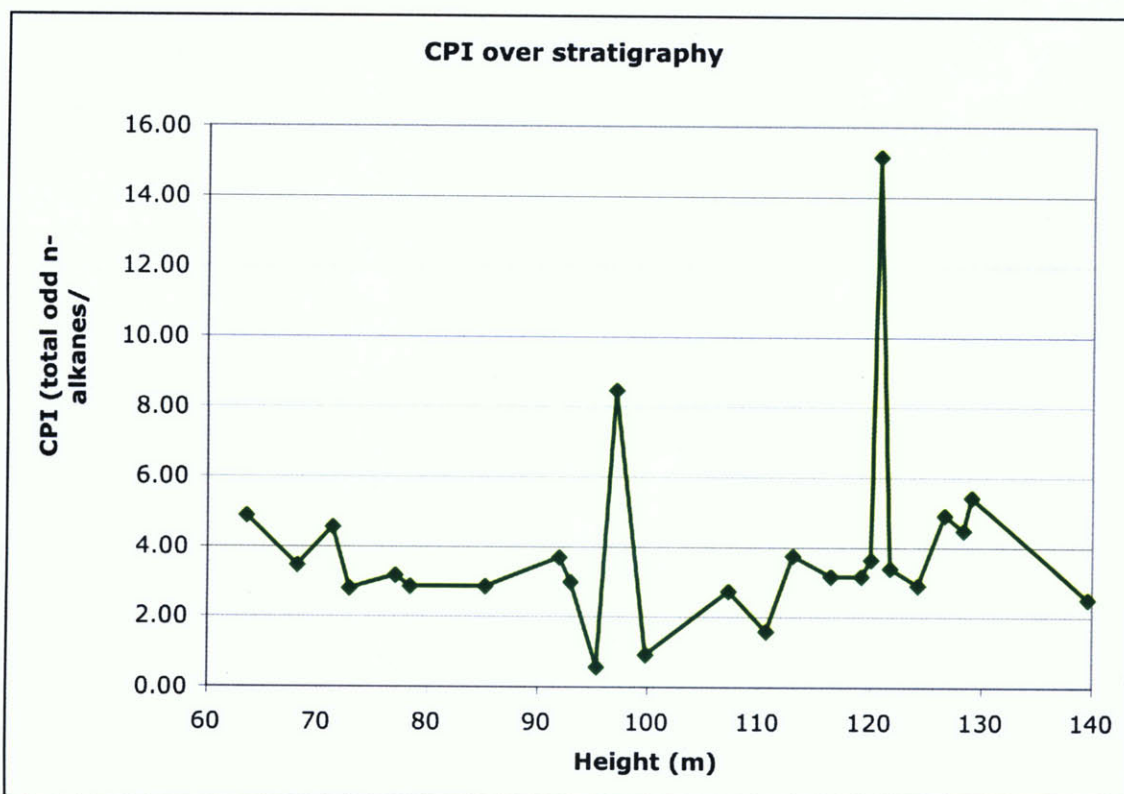


Figure 18. CPI (Carbon Preference Index) over the Axel Heiberg stratigraphy. CPI is calculated as (total concentration of odd-chain *n*-alkanes)/(total concentration of even-chain *n*-alkanes).

One final way to illustrate floral input is by calculating CPI, or Carbon Preference Index (Figure 18). This proxy value is the ratio of [all odd *n*-alkanes]/[all even *n*-alkanes] in a given sample. All values shown indicate an odd-over-even predominance, ranging from 0.57 in the C layer (at 95.4m) to 15.13 in the M layer (at 120.73m). Notably, also, in

the E layer at 100m, CPI reaches the second-lowest value of the entire record (0.93). This record tells us little more than that odd-chain *n*-alkanes are generally favored in this sediment record, indicating thermal immaturity and diagenetic decarboxylation of the original even-chained precursors (Zavarin and Cool 1981).

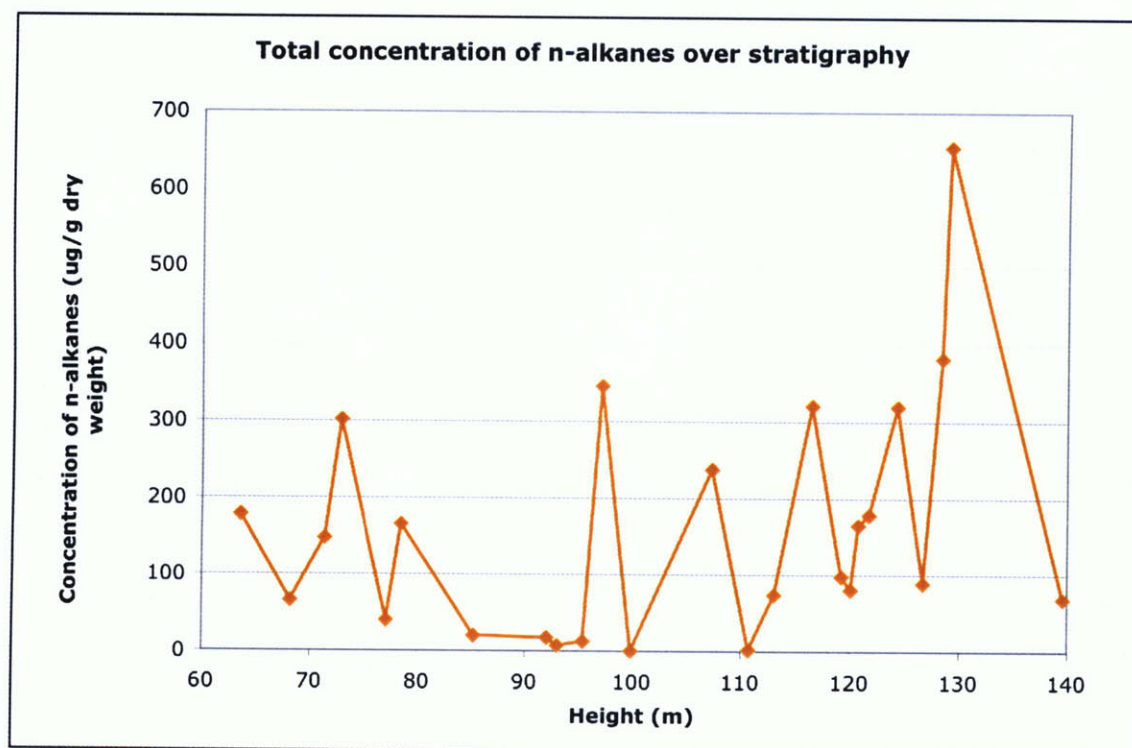


Figure 19. Normalized abundance of all *n*-alkanes in the Axel Heiberg stratigraphy.

To further inform the data presented in Figures 16-18, Figure 19 shows the normalized abundance of *n*-alkanes in each layer. Note that in the E layer (~100m), where extremes of CPI and P_{aq} are observed, the abundance of *n*-alkanes was markedly low. Therefore, the anomalous values may simply be an artifact of low abundance, with little statistical significance. The H layer may be treated with similar suspicion, given its

low *n*-alkane abundance. On the other hand, abundance in the M layer is low, but extant. Overall, the records of *n*-alkane abundance and CPI do not significantly correlate ($R^2=0.09$), indicating that but perhaps for a few isolated cases, the observed *n*-alkanes faithfully record the diversity of existing flora, regardless of abundance in the layer.

Raw abundances may further illuminate two parameters: floral input and fidelity of preservation. If *n*-alkane abundance reflects the former, we observe vacillations of the amount of extant flora, which are reflected in the record, e.g. successions of forest types. If *n*-alkane abundance reflects the latter, we observe vacillating conditions under which preservation was possible, e.g. more or less acidic burial. The two may or may not be mutually exclusive; that is, the vacillations observed in the record may be a product of one or both parameters.

Basinger (1991) observed a general decrease in diversity and abundance of plant fossils, based on macrofossil assemblages, upward through the stratigraphy. This correlates roughly with the data in Figure 19. This worker and also LePage (2003) observed a slight prevalence of Pinaceae (e.g. *Tsuga* and *Picea*) upwards, as well, which may indicate a shift to cooler temperatures, under which temperature-sensitive species would have perished. Ricketts (1991) classified the entire sequence as one biostratigraphic unit, based on shifting pollen assemblages that were not confined to one lithological type, indicating that these assemblages were recorded faithfully in spite of preservation conditions. Therefore, assuming that lipids are faithfully preserved under the same conditions pollen is faithfully preserved, we favor the explanation that the fluctuating *n*-alkane abundances observed in Figure 19 are attributable to fluctuating abundance of extant flora, rather than fluctuating preservation conditions.

Compound-Specific Hydrogen Isotopes

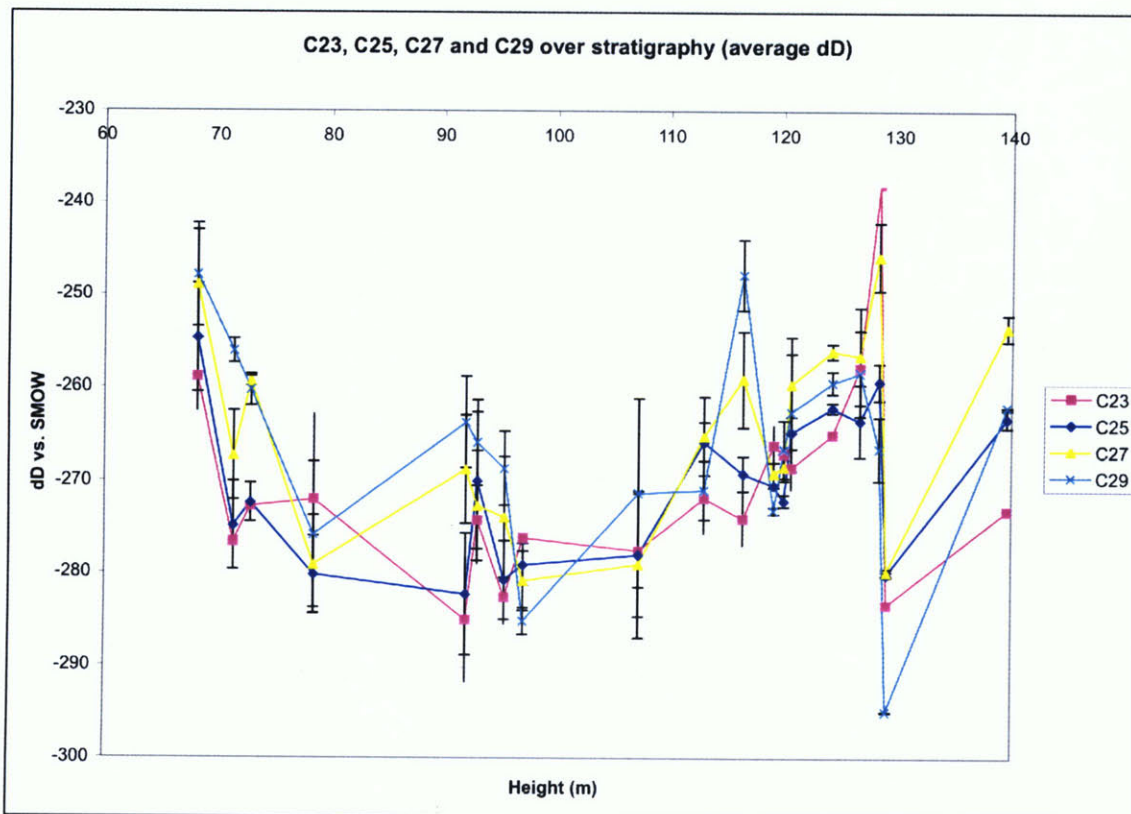


Figure 20. δD vs. SMOW of individual *n*-alkanes, C₂₃, C₂₅, C₂₇ and C₂₉, over the Axel Heiberg stratigraphy. Error bars represent error due to 1) multiple measurements and 2) correction for calibration to one peak.

The stratigraphy of *n*-alkane hydrogen isotopes is shown in Figure 20. Time moves from right to left, from old to young. The data trend from heavier to lighter isotopes over time, with large shifts balking this trend near the oldest and youngest layers of the stratigraphy. Sessions (1999) noted that *n*-alkanes generally become more enriched with longer chain lengths, a trend which is slightly observed in our data. It should also be noted that the averaged hydrogen isotope signal, taken from the data shown in Figure 20, shows no correlation ($R^2=0.0004$) with the carbon isotope signal shown in Figure 14.

This is not unexpected, given that for plants, the provenances of source water (precipitation and ground water) and organic carbon (atmospheric carbon dioxide) are governed by separate climatic parameters that are not directly linked.

The record of secular change can be more easily visualized in Figure 21, which averages the data in Figure 20.

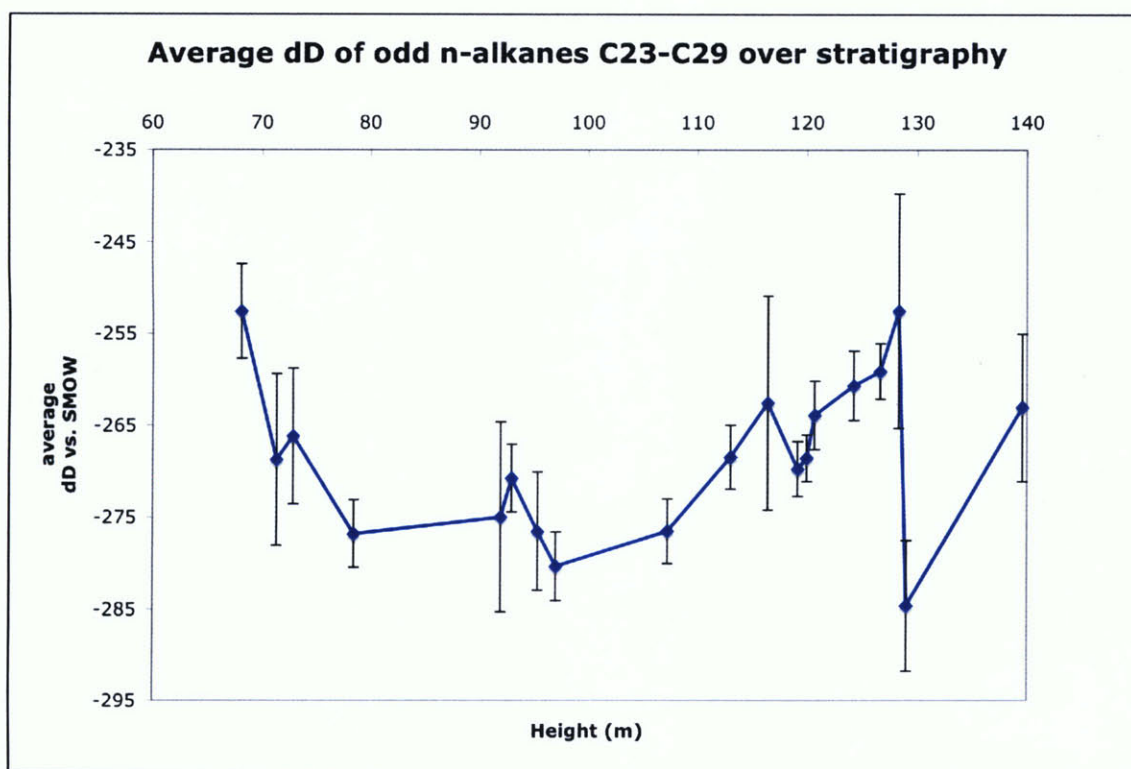


Figure 21. Average δD of odd n -alkanes from C_{23} - C_{29} (data in Figure 20). Error bars represent error due to 1) multiple measurements and 2) correction for calibration to one peak.

Hydrogen isotopes are often used to reconstruct paleohumidity. From analyzing cellulose δD and $\delta^{18}O$ in tree stumps excavated at the F layer, Jahren (2003) showed that

Eocene relative humidity (RH) was about twice the modern value (67% RH vs. 33% RH), with predicted environmental oxygen isotopes ranging from -25‰ to -12.5‰ and cellulose hydrogen isotopes ranging from -227.5‰ to -108.75‰.⁶ However, the most reasonable value for $\delta^{18}\text{O}_{\text{environmental}}$ should correlate with the deduced Eocene GMWL, $\delta\text{D} = 9.5\delta^{18}\text{O} + 10$, so we choose -15.1‰ as $\delta^{18}\text{O}_{\text{environmental}}$, and thus $\delta\text{D}_{\text{environmental}} = -133.45\text{‰}$ (see figures in Jahren 2003 and Jahren and Sternberg 2002 for illustration of these calculations).

To see what estimate our current data reveal, we need to establish a value for $\epsilon_{\text{n-alkanes/water}}$. Sessions (1999) reported $\epsilon_{\text{n-alkanes/water}}$ to be ~160‰, but these were empirical studies based on culture growth wherein environmental humidity was not recorded. Sauer (2001) reported widely varying $\epsilon_{\text{n-alkanes/water}}$ of -80‰ to -165‰ for *n*-alkanes of terrestrial or mixed origin. Though our *n*-alkanes are also of mixed origin, the data presented in Figure 20 come from higher, terrestrial plants only.

Chikaraishi (2003) reported that $\epsilon_{\text{n-alkanes/water}} = -116 \pm 13\text{‰}$ (Chikaraishi 2003) in higher plants; conifers, to be specific. Furthermore, the data were taken from trees in Japan and Thailand, where relative humidity is comparable to that calculated for the Arctic Eocene, 67%. The yearly average relative humidity is 73% for Bangkok and 68% for Tokyo (Weatherbase 2005).

The average δD of our data for higher plants is $-268.2 \pm 10.4\text{‰}$. Therefore, using the $\epsilon_{\text{n-alkanes/water}}$ provided by Chikaraishi (2003), our calculated $\delta\text{D}_{\text{environmental}} = -152.2\text{‰} \pm 23.4\text{‰}$. This value agrees with the cellulose estimate by Jahren, $\delta\text{D}_{\text{environmental}} = -133.45\text{‰}$ (2003).

⁶ These values were calculated by the assumed Eocene GMWL $\delta\text{D} = 9.5\delta^{18}\text{O} + 10$ (Jahren 2003).

Today, the δD value of precipitation in the Axel Heiberg locale is approximately -220‰ (Bowen 2003) or -212.5 +/- 7.3‰ (Global Network of Isotopes in Precipitation) as measured at Resolute Bay, at 74.72 N and -94.98 E. This value for precipitation, however, should not be confused with the value for Axel Heiberg Island's environmental water, the modern value for which is not known. We also do not know the isotopic value of Eocene precipitation, though we know it made a contribution to environmental water, whose signature manifests in cellulose.

Eocene cellulose is significantly depleted in $\delta^{18}O$ relative to modern cellulose. Jahren and Sternberg (2002) suggested that this low value was the result of isotopically depleted precipitation, coupled with warm temperatures. This combination was inferred to be the result of meridional weather patterns. In other words, cloud masses moved northeastwards from the Pacific, across North America (refer to Figure 1). In modern times, this movement is prevented by the Polar Front, an interface that separates tropical air masses from polar air masses. In the absence of a Polar Front, moisture moving across continents would have become increasingly depleted in the heavy isotope. Therefore, according to this hypothesis, moisture arriving at Axel Heiberg Island in the Eocene would have been significantly depleted in deuterium relative to modern precipitation.

Pronounced seasonality is another possible cause for the Eocene depleted cellulose. Currently, proxy data indicate that temperatures did not drop below freezing in the continental interiors (Greenwood 1995), and models have been constructed to explain this (Sewall 2004, Sloan 1998, Sloan 2001, Upchurch 1998). However, Basinger (1991) noted that the preserved tree stumps lacked late wood, a relatively hard accretion that occurs in response to frost. Today, there is an ice cap on the Princess Margaret Arch (see

Figure 1, west of fossil forest site), but it is difficult to constrain the Eocene topography. Therefore, there is no current evidence to support the hypothesis that snowmelt contributed to environmental water. However, condensation at lower temperatures also depletes precipitation of deuterium. It is possible that colder winter temperatures, still above freezing, had enough of an effect to cause the observed isotopic depletion in Eocene cellulose.

Not only is there a discrepancy between ancient and modern values, but there are large fluctuations within the ancient record itself. Wade (2002) observed fluctuations of lesser, but still high, magnitude in $\delta^{18}\text{O}$ of both planktonic and benthic foraminifera in the middle to late Eocene. The fluctuations occurred repeatedly in as little as 3 kyr, over a period of 2.3 million years.

Wade attributed these fluctuations to nascent ice volume effects, though this would only account for a shift of 9‰ in hydrogen isotopes of ocean water (Lear 2000). The required shift in salinity is considered far too big (at least 4-10 ppt) to be a reasonable option. The only remaining option is fluctuating temperature. Wade (2002) calculated that shifts of $>10^\circ\text{C}$ had to occur to produce the observed $\delta^{18}\text{O}$ shifts. These are enormous shifts, and the time scale on which they might have occurred is of utmost importance.

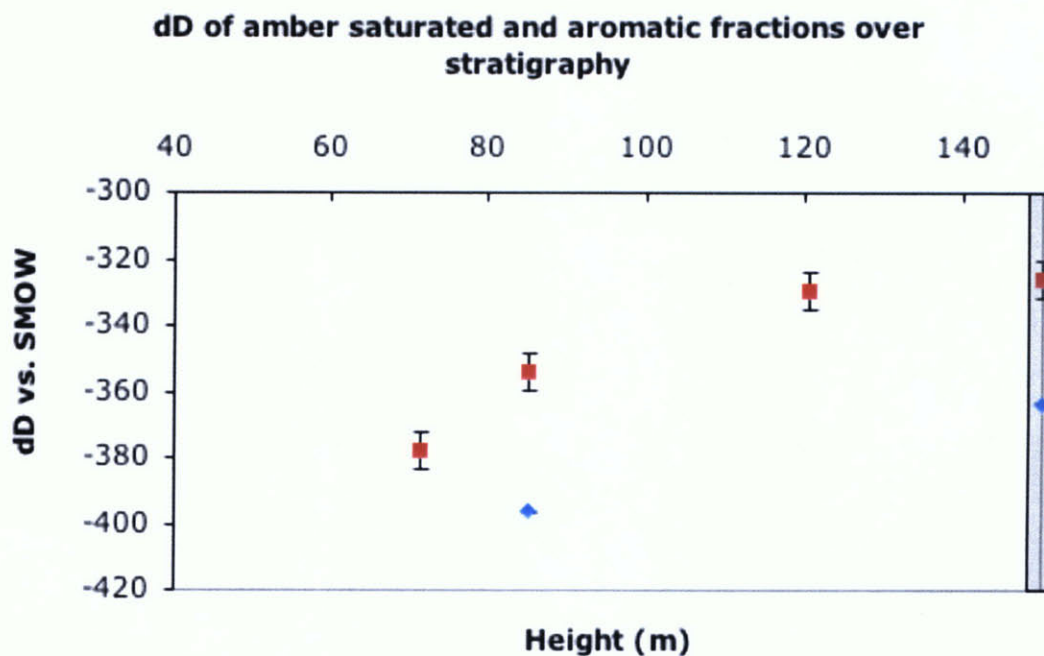


Figure 22. δD of saturated and aromatic fractions of pure resinite. From left to right, the layers are G', B' and M, or youngest to oldest through the stratigraphy. The right-most point, shaded in grey, represents mixed resinite collected from all over the site.

Figure 21 shows bulk δD of saturated and aromatic fractions of pure resinite, collected from the G', B' and M layers, as well as a composite of resinites collected from all over the site (shaded grey box). Previous values for $\delta D_{\text{resinite}}$, collected from Eocene through Miocene sediments, have ranged from -167‰ to -272‰ (Nissenbaum and Yakir 1995). Our data show lipids far more deuterium depletion than those previously reported, while carbon isotopes are approximately the same.

Our data also show a trend towards lower δD values over time. This trend parallels the trend in the corresponding leaf *n*-alkanes, though there are only two intervals where both data were measured (see Figure 19).

There is also a gap between the saturated and aromatic fractions. The aromatic fraction is approximately 40‰ heavier than the saturated fraction. It is possible that exchange with environmental water occurred during diagenetic aromatization of the labdanoid monomers, which is known to occur in resins not subject to high thermal stress. It is also possible that the resin occluded phloem or xylem upon exudation, which would have introduced less depleted carbohydrates and stem water, respectively (Anderson and Crelling 1995).

Still, in keeping with these previous observations, both the saturated and aromatic fractions of resinite are more heavily depleted than leaves (Table 5). This is partially due to the fact that gymnosperm resinites' extractable monomers are C₂₀ labdanoids (Anderson and Crelling 1995), i.e. isoprenoids made by the MEP pathway. For deuterium, the MEP isoprenoid pathway has a much greater depletive isotopic effect than the acetogenic pathway (Hayes 2001), which explains why the resinite bulk lipids are so deuterium-depleted compared to their leaf-borne *n*-alkane counterparts (Table 5).

	$\Delta\delta\text{D alk-sat}$	$\Delta\delta\text{D alk-aro}$
G' layer	n/a	109.03
B' layer	n/a	n/a
M layer	n/a	76.43
Mixed	97.69	60.18

Table 5. Comparison of δD of leaf-derived acetogenic *n*-alkanes vs. δD of resinite-derived isoprenoids, both saturated and aromatic. Resinite samples came from *in situ* tree stumps from the indicated lignite layer. "Mixed" represents resinite collected from all over the site. Half of the data is not available due to low abundance of *n*-alkanes or lack of extractable saturated fractions from resinite.

Given the complexity of resinite synthesis versus the straightforwardness of *n*-alkane biosynthesis, the latter represents a more sound approach to calculating $\delta D_{\text{environmental water}}$. Therefore we will not attempt an estimate of $\delta D_{\text{environmental water}}$ using resinite δD values.

Polycyclic lipids were also isolated from the *nab* and *nac* fractions of layers C, P, R, S and H'. The layers were chosen because they exhibited relative extremes in the δD record. These lipids were identified by GC-MS analysis and quantified by GC-FID analysis in preparation for analysis by the GCIRMS. For reasons still unknown, even though concentrations were precisely calculated to ensure sufficient abundance, the peaks of individual compounds rarely reached the 1000 mV necessary for a reliable signal.

This quandary prompted an investigation into the mass dependence of isotopic readings on the GCIRMS. First, because the isotopic values of the peaks in the standard Arndt A are known, data were collected on Arndt A peaks ranging from 105 mV to 6458 mV. The results are shown in Figure 23.

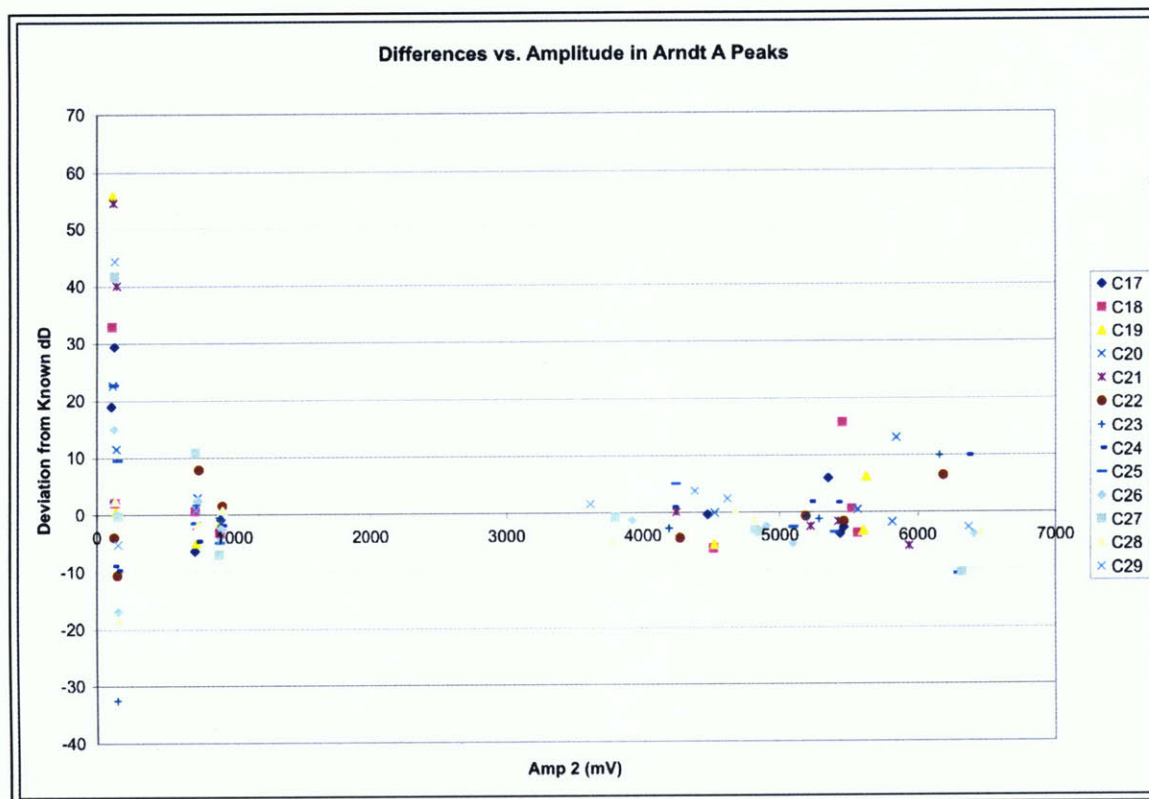


Figure 23. The Arndt A standard consists of fifteen peaks, C_{16} - C_{30} all, whose isotopic values are known. The middle peaks are calibrated to the bracketing peaks, C_{16} and C_{30} . This graph shows the deviation of these peaks' isotopic values as a function of their amplitude.

The graph shows a wide scatter at amplitudes below 500 mV, coalescing around 1000 mV and 4000-5400 mV. Scatter increases beyond 5500 mV.

The data shown may well not be only a function of amplitude. Several other factors may contribute to instrument performance from day to day. In any case, Figure 23 does not provide a clear function to which we can correct the low values of the compounds in the *nab* and *nac* fractions.

As another option, the same data were collected for ten *naa* lignite fractions, chosen because the amplitude range of their C_{29} peaks (over several trials) span 188 mV

to 15647 mV. The relationship of amplitude to isotope value was always logarithmic, as shown in the example of the A layer, in Figure 24.

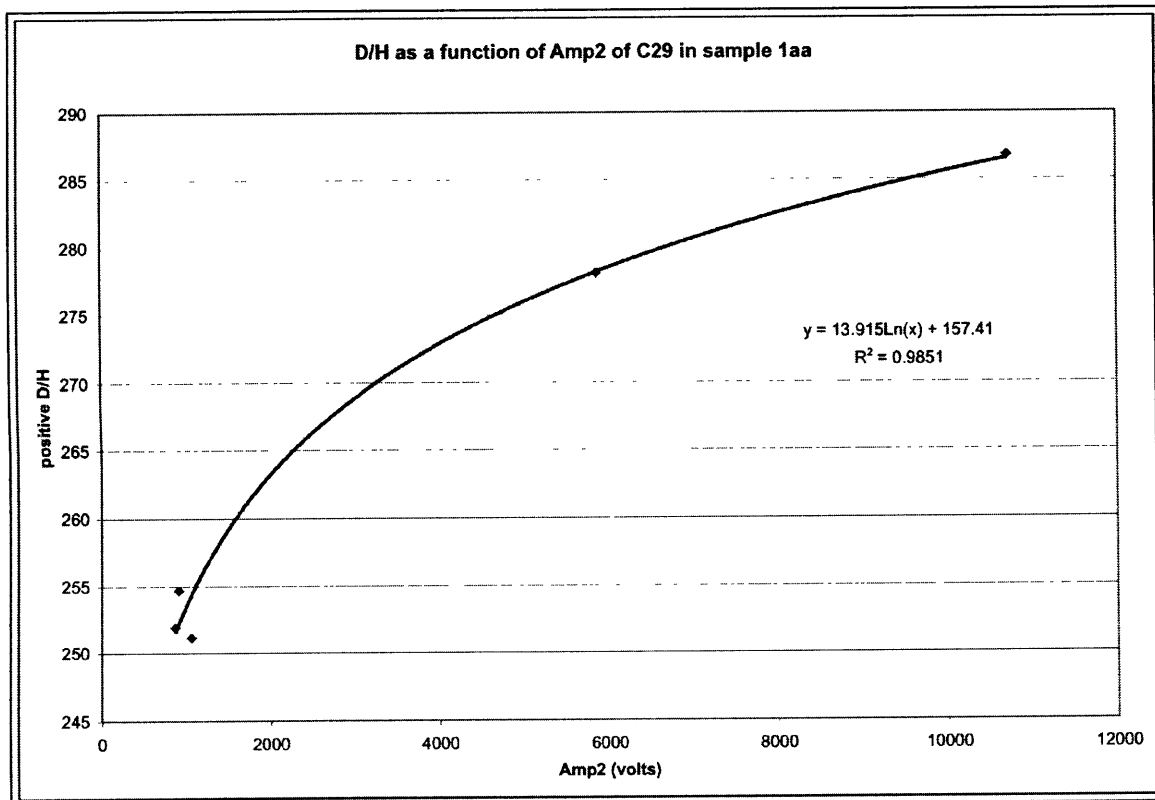


Figure 24. δD of the compound C_{29} in the same sample (A layer lignite) as a function of peak amplitude on the mass spectrometer.

The relationship is not always as well-defined as this one. The average R^2 value for all of the functions is 0.7782 ± 0.28 . The average slope of all ten logarithmic curves is 13.2 ± 6.2 . (Note: the y-intercept will be different for each sample, because δD of C_{29} in each sample is expected to be different.)

But if only the functions with $R^2 > 0.8$ are counted (mean $R^2 = 0.9402 \pm 0.0526$), the average slope is 16.5 ± 5.6 . Because the relationships upon which this datum is based are more statistically sound, we prefer it for the following calculations.

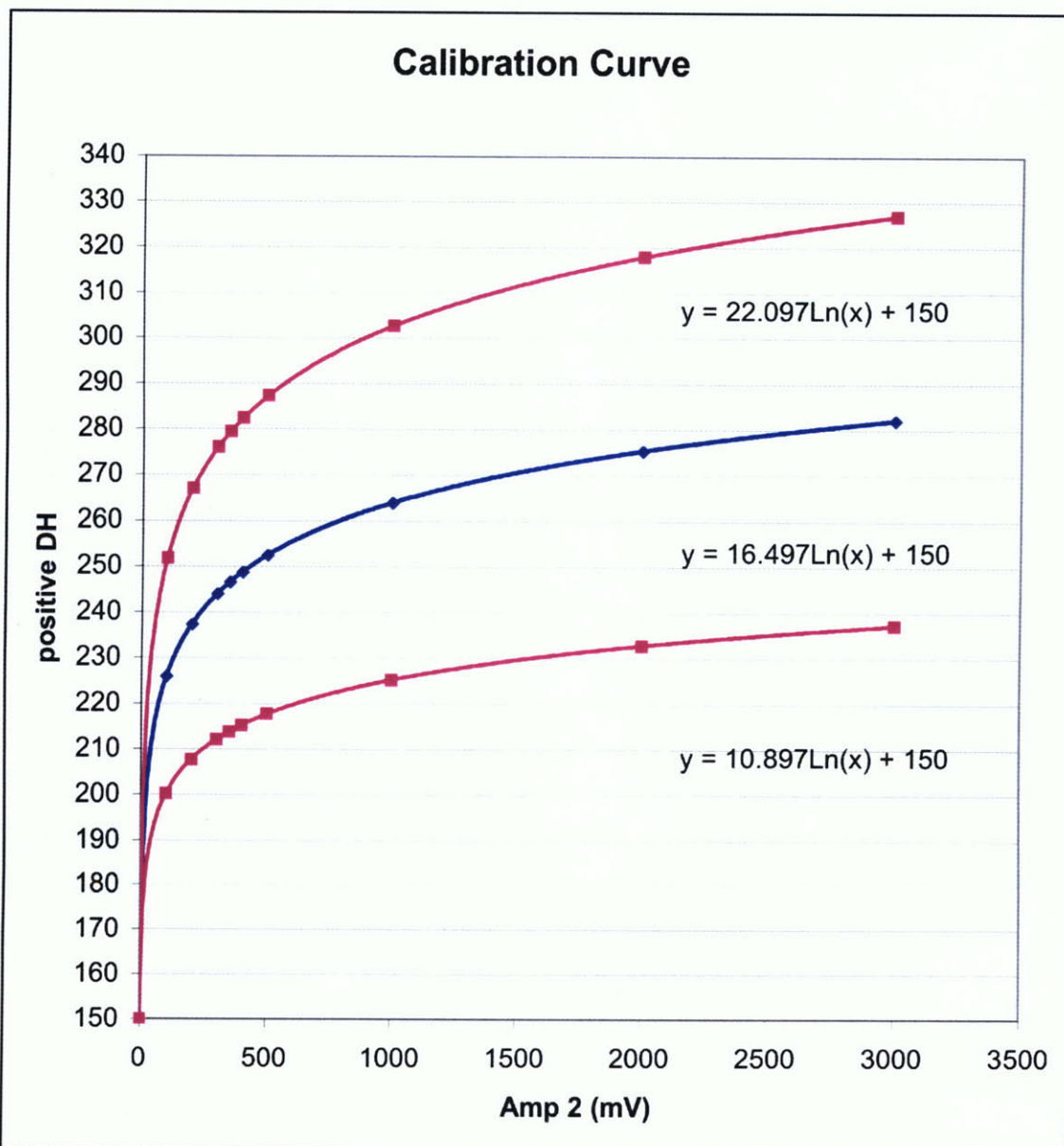


Figure 25. Calibration curve for correction of low-amplitude peaks. The slope of the blue function represents the average of the slopes of six logarithmic functions generated by plotting δD vs. amplitude for the C_{29} peak. The R^2 value of each of the original functions was > 0.8 . The pink lines represent the error of that slope (± 5.6).

We applied this correction to the isotopic values of the *nab* and *nac* fractions' compounds. That is,

$$\delta D_{\text{corrected}} = 16.4973(\delta D_{\text{measured}}) - (\ln(\text{actual amplitude}) - \ln(2000\text{mV})) \quad (5)$$

We chose 2000 mV as the standard amplitude because it marks the beginning of the flat portion of the logarithmic curve. That is, error is smaller than at 1000 mV.

An additional correction was applied to account for calibration to C₁₆ alone, as opposed to C₁₆ and C₃₆ together. The correction carried an error of no more than 3.3%.

These corrections resulted in the following data set.

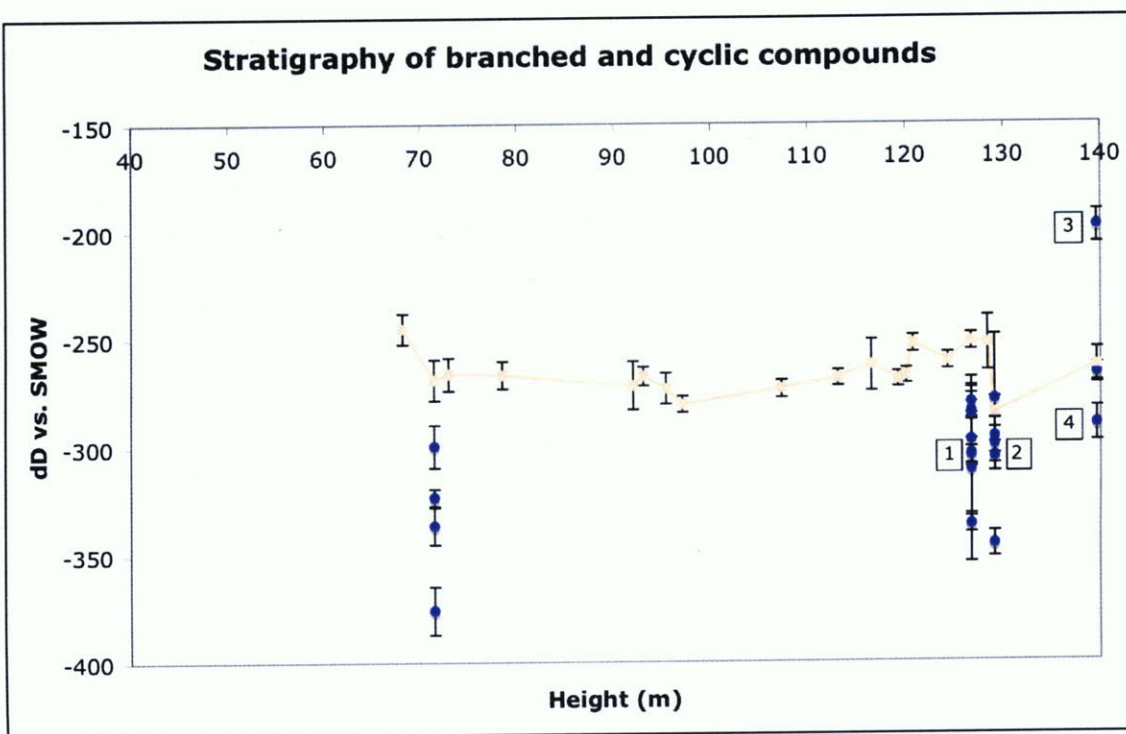


Figure 26. Compounds from the *nab* and *nac* fractions, eluted from the original hydrocarbon fraction with 25% ethyl acetate and 100% ethyl acetate, respectively. (They are not distinguished on the graph.) Blue points denote individual compounds. 1) simonellite, 2) 17 α (H)-bishomohopane, 3) dehydrobietane, 4) homohop-17(21)-ene or 17B(H)-homohop-29(31)-ene. The others are unknown polycyclic terpenoids. The pink series is average δ D of *n*-alkanes for comparison.

Figure 26 shows, in blue, the hydrogen isotope values of individual polycyclic terpenoids. The pink series shows average *n*-alkane values for comparison. Four polycyclic compounds have been tentatively identified:

1) simonellite at -303.77‰, which is a biomarker for higher plant input, especially conifer resin (e.g. Jiang 1998, Staccioli 2002),

2) 17 α (H)-bishomohopane at -295.72‰, a bacterial biomarker (e.g. Ourisson 1979),

3) dehydroabietane at -198.19‰, a biomarker for higher plant, especially conifer, resin (e.g. Schulze 1990, Tuo 2003),

4) homohop-17(21)-ene or 17 β (H)-homohop-29(31)-ene at -289.86‰, a bacterial biomarker (e.g. Ourisson 1979).

Chikaraishi (2004b) demonstrated that, in *Cryptomeria japonica* (a model C3 gymnosperm), lipids are depleted according to their synthesis by one of three pathways. The acetogenic pathway produced *n*-alkyl lipids depleted relative to environmental water by 91-152‰. C₁₅ and C₃₀ isoprenoid lipids produced by the MVA pathway were depleted relative to environmental water by 212-238‰. C₂₀ isoprenoid lipids produced by the MEP pathway were depleted 238-303‰ relative to environmental water. Table 6 shows the calculation of $\delta D_{\text{environmental water}}$ based on these parameters.

None of the estimated values for $\delta D_{\text{environmental water}}$ approach the value derived from *n*-alkanes previously in this paper. Also, estimates from the same layer (S layer, in green) are very different, with $\delta D_{\text{environmental water}}$ from dehydroabietane an unlikely positive value. Because of the uncertainty in compound identification, we do not recommend estimation of $\delta D_{\text{environmental water}}$ from the polycyclic compounds presented here.

Layer	Compound (?)	dD	Environmental water dD	
			Low extreme	High extreme
P	simonellite	-303.77	-65.77	-0.77
R	17A(H)-bishomohopane	-295.72	-83.72	-57.72
S	dehydroabietane	-198.19	39.81	104.81
S	17B(H)-homohop-29(31)-ene	-289.86	-77.86	-51.86

Table 6. Estimation of $\delta D_{\text{environmental water}}$ based on isotope fractionation parameters in Chikaraishi (2004b).

Assuming common source water, we would expect an offset of about 60‰, minimum, between *n*-alkanes and isoprenoids. This is not always observed in the data in Figure 26; there is no consistent offset, though the expected offset falls within the ranges shown in Table 7. Grouping the isoprenoids into C₁₅-C₃₀ and C₂₀ groups also does not produce the expected offset (data not shown).

	Average <i>n</i>-alkane - isoprenoid	Stdev.
G' layer	65.05	41.33
P layer	48.56	22.42
R layer	20.28	31.93
S layer	-11.60	55.65

Table 7. For each layer where isoprenoid isotope information is available, the offset between average isoprenoid and average *n*-alkane values within a given layer. Standard deviation is the pooled standard deviation of the average *n*-alkane value and the average isoprenoid value.

This lack of offset is probably explained by the fact that the error bars are simply too large to allow an accurate comparison.

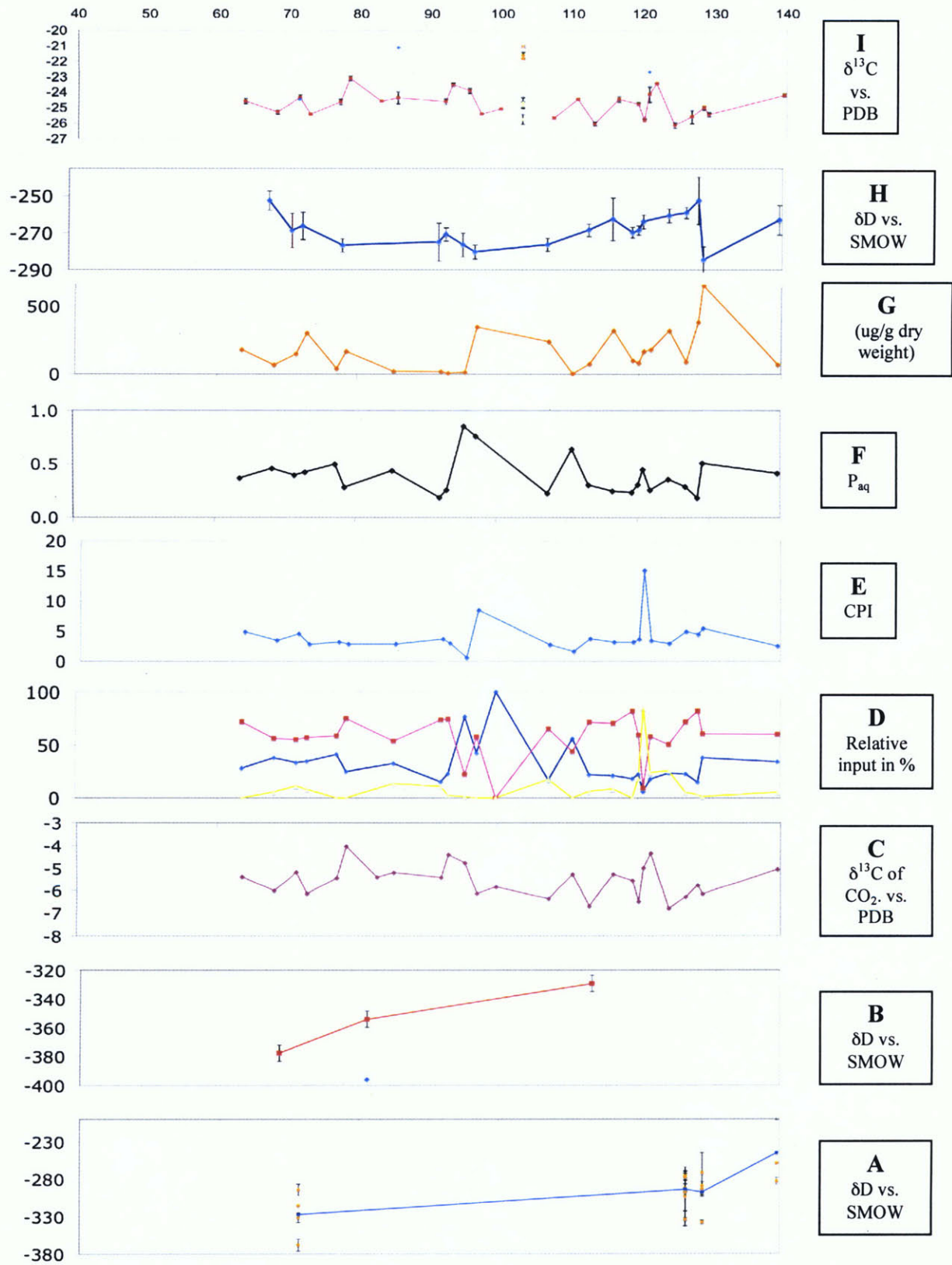
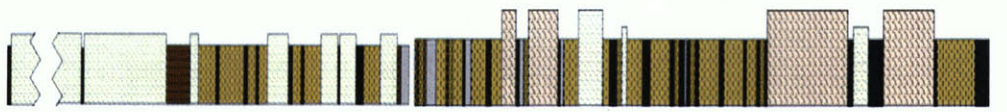


Figure 27. Comparison of all previously discussed records over the Axel Heiberg stratigraphy. Note: data do not exist for layers above 40m. (A) δD of polycyclic compounds. Orange points represent individual compounds and the blue line represents the average for that layer. (B) δD of resinites. Red points represent the aromatic fraction and the blue point represents the saturated fraction. (C) $\delta^{13}CO_2$ of the atmosphere as calculated by Equation (3). (D) Relative input of different odd n -alkane groups. Blue represents $\%C_{21}-C_{25}$. Red represents $\%C_{27}-C_{31}$. Yellow represents $\%C_{33}-C_{35}$. (E) Carbon Preference Index, the total concentration of odd over even n -alkanes. (F) P_{aq} , the measure of proportional contribution of aquatic plants. (G) Total $\mu g/g$ dry weight of n -alkanes in that layer. (H) Average δD of odd n -alkanes $C_{23}-C_{29}$. (I) Bulk carbon $\delta^{13}C$. Red represents lignites. Blue represents resinite. Orange represents wood. Yellow represents paleosols.

The various records described above are presented in Figure 27, aligned to the stratigraphy. Since it is difficult to draw definitive conclusions from curve shapes alone, we performed a statistical analysis of the data. Records not derived from the same data set were compared to each other. Of the records that were explicitly related to each other, i.e. derived from the same data set (such as $\delta^{13}C_{atmosphere}$ and bulk lignite $\delta^{13}C$), the less derived record was chosen.

Furthermore, the resolution of data was not consistent from record to record. For example, a particular layer may have a data point for bulk $\delta^{13}C$ but not for δD . When there are gaps in the data, there are two options. We can 1) extrapolate the missing data linearly from established points or 2) analyze only the layers for which all data are available. Experience with these samples has shown that finer resolution usually means greater fluctuation, so that extrapolation would lead to aliasing. For that reason, even though many data will be thrown out, we believe it would be better to analyze only the layers for which all data are available.

The data sets selected for analysis were: δD , P_{aq} , CPI, concentration, bulk $\delta^{13}C$, and $\%C_{27}-C_{31}$. First, each of the records was compared against each other in a simple

correlation analysis, resulting in a Pearson Product moment correlation coefficient. These R^2 values represent how much of the variance in one data set can be attributed to the other; i.e., the correlation. As seen in Table 8, none of the records had an especially strong correlation with each other. The only possible exception is P_{aq} and $\%C_{27-31}$, which show a weak anti-correlation of -0.6701. This may be expected because the former is a proxy of aquatic plant input, and the latter is a proxy of higher terrestrial input. So, they manipulate the same data in different ways to arrive at the same parameter, which explains their weak anti-correlation.

	δD	P_{aq}	CPI	conc.	blk $\delta^{13}C$	$\%C_{27-31}$
δD	1.0000	-0.3387	0.1803	-0.2595	0.0362	-0.0253
P_{aq}	-0.3387	1.0000	0.1484	0.0977	0.0402	-0.6701
CPI	0.1803	0.1484	1.0000	0.2061	-0.0451	-0.4821
conc.	-0.2595	0.0977	0.2061	1.0000	-0.2625	0.0523
blk $\delta^{13}C$	0.0362	0.0402	-0.0451	-0.2625	1.0000	-0.1805
$\%C_{27-31}$	-0.0253	-0.6701	-0.4821	0.0523	-0.1805	1.0000

Table 8. Pearson product moment correlation coefficients of each pair of the data sets presented in Figure 27.

To make sure the signals were unrelated, the matrix of the six records presented above was analyzed with empirical orthogonal functions (EOF). Each data set was normalized by its own standard deviation to give the corresponding vector unit length. Also, the mean was subtracted from each data set to prevent biasing towards data sets that featured means of large magnitude.

The results showed that ~56% of the variance could be explained by the first two vectors, ~76% by the first three, and ~88% by the first four. In other words, the records are demonstrably unrelated.

Having presented the isotopic records, it is crucial to now consider the time scales on which the fluctuations occurred. The lignite layers are always separated by layers of clay, sandstone, organic-rich shale, and mudstone (see Figure 7). In addition, the lignite layers vary considerably in thickness, from 0.1 meters to 3.0 meters (Hagopian, pers. comm.).

Kojima et al (1998) devised a method to calculate the accumulation rates of these lignite layers based on the assumption that the Leaf Area Index, or LAI (the ratio of tree leaf area to ground surface area) was mostly constant during the time of deposition. In other words, a deciduous tree will produce about the same amount of leaf area every year, which will, in turn, cover about the same amount of space on the ground when the leaves fall in autumn.

Since the leaves found in the Fossil Forest are so well preserved, it was possible to measure the surface area of the leaves. The leaves of the N layer were chosen for analysis. LAI for *Metasequoia* is more difficult to measure, given the extreme rarity of modern stands. Therefore, LAI was estimated from a selection of deciduous trees, both conifers and broad-leaved angiosperms (Kojima 1998, data from Cannell 1982). The age of the stand matters more than the species of tree. Scatter is considerable up to, and including, stand age=150 years. *Metasequoia* individuals from the F layer were 50-75 years old when they died (Jahren 2004). Since LAI only begins to level off around 100

years, there is almost certainly significant error with the assumed LAI in this study. For this reason, we report ages calculated from the minimum (LAI=5, the composite of deciduous conifer and broadleaved species) to the maximum (LAI=8.5, the sole data point for LAI of *Metasequoia*).

Accumulation rate was thus calculated according to the following equation:

$$x = (L S D)/(r W) \quad (10)$$

where x = accumulation rate (in cm/year), L = LAI (in year⁻¹), S = surface area of stand or sample taken (in cm), D = lignite layer thickness (in cm), r = surface area/weight ratio (in cm²/g), and W = weight of sample (in grams). (Kojima 1998)

Extrapolation of this value to all the lignite layers is justified by two data. First, *Metasequoia* leaves dominate all of the lignite layers (Basinger 1991). Second, *Metasequoia* has remained evolutionarily static (at least in terms of morphology) since the Cretaceous and so, we assume, within a small interval in the Eocene as well (LePage 2005).

Extrapolation of this value to all lignite layers is undermined by several other considerations. First, since the calculations were only done on one layer, the value of r must be assumed for all layers. Second, the method is only applicable to leaf lignites; there were no recognizable leaf fossils in our lignite samples, though we are assuming the material is leaf-derived. This means that we assume leaf area to be constant in time. Also, we have no record of the surface area of the stand, or, more specifically, the sample taken; density is unknown. Finally, we assume that the lignite material is derived solely

from *Metasequoia*, which could well not be the case, given that other taxa are present (Basinger 1991) and that leaves of different taxa decompose differentially (Elder and Cairns 1982).

Having said all that, application of the accumulation rate 0.8 mm/year to all layers results in minimum layer ages ranging from 125 years to 3750 years. Altogether, then, the lignite layers represent a minimum time span of ~18,000 years (Table 9). Of course, as stated before, the lignite layers occur only intermittently between clastic layers, the ages of which have not been determined. Therefore, the intervals of time between successive lignite layers remain unknown.

Layer	Thickness (m)	Duration (yrs)
K'	0.15	187.5
J'	0.15	187.5
I'	3	3750
H'	0.3	375
G'	0.4	500
F'	0.3	375
E'	0.5	625
D'	0.3	375
C'	0.2	250
B'	0.6	750
A	0.3	375
B	0.1	125
C	0.25	312.5
D	0.1	125
E	0.5	625
F	0.4	500
G	0.2	250
H	1.5	1875
I	0.7	875
J	0.8	1000
K	0.5	625
L	0.3	375
M	0.3	375
N	0.4	500
O	0.5	625
P	0.1	125
Q	0.1	125
R	0.1	125
S	1.3	1625

Table 9. Known thickness of each lignite layer, and extrapolated deposition time span, based on the methodology described by Kojima (1998).

Using Equation (10), it is also possible to calculate accumulation rates for each of the layers, though in our case there is one unknown, S (the surface area of the sample taken). Therefore, all resulting deposition times are scaled to S (see Table 10). The minimum and maximum deposition times are based on the estimates of LAI=8.5 (the sole

data point for *Metasequoia*, from a modern stand) and LAI=5.0 (the average of many LAIs for deciduous conifers and broad-leaved trees; see Kojima 1998), respectively.

Layer	Minimum Deposition Time (years) x S	Maximum Deposition Time (years) x S	Unknown (sample area)
I'	59.1	100.5	x S
H'	44.1	75	x S
G'	61.5	104.5	x S
F'	62.8	106.8	x S
E'	59.9	101.9	x S
D'	63.8	108.4	x S
B'	59.0	100.3	x S
A	50.8	86.4	x S
B	61.3	104.2	x S
C	59.9	101.9	x S
D	42.1	71.6	x S
E	58.9	100.1	x S
G	28.8	49	x S
H	61.4	104.4	x S
I	67.3	114.4	x S
J	48.1	81.8	x S
K	59.8	101.7	x S
L	59.1	100.4	x S
M	64.2	109.1	x S
N	60.1	102.1	x S
O	57.1	97	x S
P	62.2	105.8	x S
Q	25.6	43.5	x S
R	60.6	103	x S
S	60.9	103.6	x S

Table 10. Minimum and maximum deposition times for each layer, using Equation (10), after methodology of Kojima 1998. Each age is scaled by an unknown factor, S, the surface area of the sample taken.

Therefore, all speculation about the magnitude and duration of climate change based on these data must be considered in light of the unknown time scale.

Rapid climate change is evident from a palynological investigation of the Axel Heiberg stratigraphy by Richter and LePage (2005). Sampling the siltstone layer between

Level O (older) and Level N (younger) coals, they found significant variability in pollen input, which was inferred to reflect climate change. Their stratigraphy was divided into five zones.

In the first zone, the level O *Metasequoia* swamp-forest appears to have been killed by a massive flooding event, after which broad-leaved deciduous flora prevailed, probably having migrated from the upstream broad-leaved deciduous floodplain. This new assemblage includes *Alnus*, which colonizes open spaces following large-scale landscape disturbance (Ritchie 1987).

The second through sixth zones feature pollen assemblages that signal a tug-of-war between drier and mesic conditions. Interestingly, in the fourth zone, an abundance of acritarchs signals the possible migration of marine elements upstream. Today, the fossil forest site is less than ten miles inland; in an ice-free world, it would have been even closer. Overall, the data indicate a dynamic ecosystem wherein vegetation was sensitive to environmental changes (Richter 2005).

Unfortunately, we do not have δD data for the O→N transition. We do have $\delta^{13}C$ data for the transition, however; carbon becomes $\sim 1\text{‰}$ heavier across the transition. The total concentration of *n*-alkanes drops slightly (see Figure 19), as does P_{aq} (see Figure 17).

On an even smaller time scale, within the N layer, Schoenhut (2005) observed an apparent oscillation in preservation of organelles within leaf cells. If the age extrapolations are to be believed, these oscillations occurred on a timescale of ~ 500 years (see Table 9).

Studies of rapid climate change in the Paleogene have mostly focused on the Paleocene-Eocene Thermal Maximum, when deep-sea temperature rose $5\text{-}6^{\circ}C$ over ca.

10^4 years (Kennett 1991). Without better age control, we cannot tell whether the fluctuations recorded in our data represent aberrational or event-scale change, 10^3 - 10^4 years (as defined by Zachos 2001). Consideration of orbital parameters is not an option, given that we don't have a continuously dated record.

Bolide impact (Kent 2003), volcanic outgassing events (Thomas 2002, Pearson and Palmer 2000), methane hydrate release (Dickens 2001), and reorganization of ocean circulation (Zachos 1993) are mechanisms that have been invoked to explain the dramatic isotopic and warming events that characterized the Paleocene-Eocene Thermal Maximum. Since our record dates from the same era, it is natural to consider the same mechanisms. Furthermore, there are no other known mechanisms for affecting temperature and carbon and hydrogen isotopes so abruptly.

Evidence of volcanic outgassing in the early Eocene was observed by Pearson and Palmer (2000), but, though looked for, none was observed for the Middle or Late Eocene. Therefore we discount this possibility as a source of warming or light carbon pulses.

While there is a chance bolide impact may have triggered methane hydrate release for the initial warm pulse of the PETM, there is little chance that multiple bolide impacts occurred. However, that initial event could have created a positive feedback, whereby warm temperatures destabilized methane hydrates, which warmed the atmosphere more.

Researchers have identified two problems with the methane hydrate hypothesis. First, why do planktonic foraminifera register the carbon and oxygen isotope excursions before the benthic foraminifera do (Thomas 2002)? Second, how could thousands of gigatons of methane escape the ocean without being oxidized?

Both these questions may be addressed by the fact that methane hydrate reservoirs do not reside in the deep ocean, but rather on continental margins where methanogens thrive in anaerobic sediments (Dickens 2001). Slope failure or widespread crystal destabilization could have resulted in several smaller methane release events. Much of this methane would be oxidized on its journey up the shallow water column. The remaining isotopically light methane reached the atmosphere, it would be quickly oxidized to isotopically light CO₂.

This light CO₂ would then have two fates. First, planktonic foraminifera would incorporate it into their shells, then die and fall into the deep ocean, where benthic foraminifera would be the secondary recipients of the light carbon. However, since the lifespan and sinking time of planktonic foraminifera is so short, this is not a satisfactory mechanism for explaining the lag time between the planktonic and benthic signals.

Second, the light CO₂ would be dispersed in the atmosphere, which has a geologically instantaneous mixing time. The light CO₂ would thus be incorporated into the terrestrial biosphere, including the biota on Axel Heiberg Island.

We should also consider mechanisms closer to the plants; that is, causes that originate *within* the Eocene Axel Heiberg ecosystem. We can discount fluctuations in floral input, because we have demonstrated that the carbon isotope signal was unrelated to the floral input signal (see Figures 15 and 18).

The “canopy effect,” whereby dense stands recycle light carbon beneath the canopy cover (Broadmeadow and Griffiths 1993), may be considered. According to Kojima (1998), the estimated LAI for the fossil forest was ~4.7-5.4. However, this estimate is based on a suite of modern deciduous conifers and broad-leaved species that

have questionable resemblance to ancient *Metasequoia* and its contemporaries. Again, the sole data point for a *Metasequoia* stand is LAI = 8.5, so there is no associated error.

Williams (2003a) recorded that the stand density of the 48-year-old *Metasequoia* plot near Tokyo, Japan is 810 trees per hectare. Williams (2003b) counted 1275 stumps per hectare in the N layer of the fossil forest. This is compared to modern cypress swamps in Alabama at 169 trees/hectare, 200-1000 trees/hectare in tropical rainforests, 1000-3000 trees/hectare in temperate broad-leaved evergreen forests, 485 trees/hectare in Finnish spruce forests, and 3000 trees/hectare in Canadian boreal needle-leaved evergreen forests (Francis 1991 and references therein).

The canopy effect increases with increasing LAI. According to the work of Buchmann (1997), for LAI = 4.5 and the deciduous species *Acer spp.*, a $\delta^{13}\text{C}_{\text{leaf}}$ gradient of approximately 4‰ is observed from the bottom to the top of the canopy (10 meters). (Discrimination is greater at the bottom, in the understory vegetation, and decreases upwards.) A lesser and more gradual gradient of 2‰ was observed for a stand of the same species with a different LAI (=2.1). No data were available for the canopy effect in stands with LAI > 4.5.

This gradient is due to two effects: (a) differences in c_i / c_a (the ratio of internal leaf CO_2 concentration to ambient atmospheric CO_2 concentration, after Farquhar 1989); and, to a far lesser extent, (b) differences in ambient CO_2 concentration along the vertical canopy profile.

According to (a), the understory of a given stand is more depleted than the overstory. That is, the understory vegetation can afford to discriminate against ^{13}C to a greater extent, either because the intracellular leaf spaces are saturated with CO_2 or the

air surrounding the leaf is. Presumably, the inter-canopy CO₂ concentrations vary to a greater extent and on shorter time scales than the above-story CO₂ concentrations do, although that question was not addressed in the study.

V. Future Work

Carbon isotopes

Questions remain. Are the carbon isotope fluctuations due to fluctuations in $\delta^{13}\text{C}_{\text{atmosphere}}$, or fluctuations in stand density? Currently there is no evidence to disprove either of these theories. This question will be constrained by two areas of research:

1) Radiometric dating. If the carbon isotopes in the lignite layers can be correlated with another middle Eocene stratigraphy that also contains ash beds, the age of the entire stratigraphy can be established, and difficulties associated with accumulation rates bypassed. We would also know more precisely the time scales on which the isotopic and floral fluctuations occurred. Dating would also enable comparison with marine records, which exist over the Middle Eocene (e.g. Huber 1999, Pearson and Palmer 2000, Zachos 1993, Bohaty 2003, Diester-Haas 1996). Wedding the marine and terrestrial records would enable unprecedented insight into the workings of the Eocene transitional period.

In lieu of radioisotope dating, the methods of Kojima (1998) could be applied to *all* layers in which preserved leaves are available. However, given the limitations outlined, this would be a less preferable method of estimating age.

2) Measure stand density for all layers that are available. These data would further constrain the effect of stand density on carbon isotope discrimination. If there is a correlation between bulk carbon isotopes and stand density, we may postulate that LAI was the primary control on plant carbon.

3) Both records would benefit from geochemical analysis at a much finer stratigraphic resolution. Each lignite sample in this study represents the bulk isotope

value for hundreds or thousands of years. Sub-sampling of the lignite layers would indicate the relative degree of secular change within a layer, even if absolute age control is absent.

Hydrogen isotopes

Time scale is also an essential issue for hydrogen isotopes. If SSTs were really shifting by 10°C on a 3 kyr time scale in the western North Atlantic, we would expect to see this reflected in the isotopic records from Axel Heiberg.

Currently, there are not enough data to favor a single climate mechanism that allowed for unusually depleted environmental water on Axel Heiberg Island in the Eocene. There are two knowns: δD of Eocene environmental water and δD of modern meteoric water on Axel Heiberg Island. There are two unknowns: δD of Eocene meteoric water and δD of modern environmental water on Axel Heiberg Island. Are the unusually depleted cellulose and leaf lipids due to meridional transport, or to seasonality? Three areas of research (besides dating) will help to constrain this issue:

- 1) Estimate the effect of seasonal cold, but still above-freezing, condensation temperatures on the isotopic composition of rain. Then calculate what contribution of this isotopically depleted rain would have been necessary to account for the magnitude of depletion observed in Eocene cellulose and leaf *n*-alkanes.

- 2) Construct climate models that specifically address the possibility of long-term meridional weather transport, and still fit with all proxy data.

3) Constrain the height of the Princess Margaret Arch in the Eocene. If topography was sufficiently developed, snow may have condensed on the uppermost slopes, contributing to isotopically depleted runoff that fed into the Eocene forest.

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References

- Abrantes, F. 2003. A 340,000 year continental climate record from tropical Africa – news from opal phytoliths from the equatorial Atlantic. *Earth Plan. Sci. Lett.* 209, 165-179.
- Anderson, K. B., and Crelling, J. C. (eds) 1995. *Amber, resinite, and fossil resins*. ACS Symposium series no. 617. Washington, DC: American Chemical Society.
- Andreasson, F. P., Schmitz, B. 1996. Winter and summer temperatures of the early middle Eocene of France from *Turritella* $\delta^{18}\text{O}$ profiles. *Geology* 24, 1067-1070.
- Arens, N.C., Jahren, A.H. & Amundson, R. 2000. Can C3 plants faithfully record the carbon isotopic composition of atmospheric carbon dioxide? *Paleobiology* 26, 137-164.
- Baas, M., Pancost, R., van Geel, B., Sinninghe Damste, J. S. 2000. A comparative study of lipids in *Sphagnum* species. *Org. Geochem.* 31, 535-541.
- Bains, S., Morris, R. D., Corfield, R. M., Faul, K. L. 2000. Termination of global warmth at the Palaeocene/Eocene boundary through productivity feedback. *Nature* 407, 171-174.
- Basinger, J. F. 1991. The fossil forests of the Buchanan Lake Formation (early Tertiary), Axel Heiberg Island, Canadian Arctic Archipelago: preliminary floristics and paleoclimate. In *Tertiary Fossil Forests of the Geodetic Hills, Axel Heiberg Island, Arctic Archipelago*, R. L. Christie and N. J. McMillan (eds.); Geological Survey of Canada, Bulletin 403, p. 39-65.
- Beerling, D. J. 1996. C discrimination by fossil leaves during the late-glacial climate oscillation 12–10 Ka BP: measurements and physiological controls. *Oecologia* 108:29–37.
- Berner, R. A. and Kothavala, Z. 2001. GEOCARB III: A revised model of atmospheric CO₂ over Phanerozoic time. *Am. J. Sci.* 301, 182-204.
- Billups, K., Schrag, D. P. 2003. Application of benthic foraminiferal Mg/Ca ratios to questions of Cenozoic climate change. *Earth Plan. Sci. Letters.* 209, 181-195.
- Bohaty, S. M., and Zachos, J. C. 2003. Significant Southern Ocean warming event in the late middle Eocene. *Geology* 31, 1017-1020.
- Bolle, M. P., Pardo, A., Adatte, T., Von Salis, K., Burns, S. 2000a. Climatic evolution on the southeastern margin of the Tethys (Negev, Israel) from the Palaeocene to the early Eocene: focus on the late Palaeocene thermal maximum. *J. Geol. Soc. Lond.* 157, 929-941.

Bolle, M. P., Pardo, A., Hinrichs, K.-U., Adatte, T., Von Salis, K., Burns, S., Keller, G., Muzylev, N. 2000b. The Paleocene-Eocene transition in the marginal northeastern Tethys (Kazakhstan and Uzbekistan). *Int. J. Earth Sci.* 89, 390-414.

Bolle, M.-P. and Adatte, T. 2001. Palaeocene-early Eocene climatic evolution in the Tethyan realm: clay mineral evidence. *Clay Minerals* 36, 249-261.

Bottomley, R., Grieve, R., York, D., Masaitis, V. 1997. The age of the Popigai impact event and its relation to events at the Eocene/Oligocene boundary. *Nature* 388, 365-368.

Bowen, G. J., and Revenaugh, J. 2003. Interpolating the isotopic composition of modern meteoric precipitation. *Water Res. Research* 39, 1299.

Bralower, T.J., Zachos, J.C., Thomas, E., Parrow, M., Paull, C.K., Kelly, D.C., Silva, I.P., Sliter, W.V., and Lohmann, K.C. 1995. Late Paleocene to Eocene paleoceanography of the equatorial Pacific Ocean: Stable isotopes recorded at Ocean Drilling Program Site 865, Allison Guyot: Paleoceanography, v. 4, p. 841-865. *ture*, v. 390, p. 497-500.

Brewster-Wingard, G.L., Scott, T. M., Edwards, L. E., Weedman, S. D., Simmons, K. R. 1997. Reinterpretation of the peninsular Florida Oligocene: an integrated stratigraphic approach. *Sed. Geol.* 108, 207-228.

Broadmeadow, M. S. J. and Griffiths, A. 1993. Carbon isotope discrimination and the coupling of CO₂ fluxes within forest canopies. In *Stable Isotopes and Plant Carbon-Water Relations*, eds. J. R. Ehrlinger, G. D. Farquhar and A. E. Hall, Ch. 8. Academic Press, San Diego.

Buchmann, N., Kao, W., Ehleringer, J. 1997. Influence of stand structure on carbon-13 of vegetation, soils, and canopy air within deciduous and evergreen forests in Utah, United States. *Oecologia* 110, 109-119.

Campbell, N. A., Reece, J. B., Mitchell, L. G. 1999. *Biology*. 5th edition. Reading, Massachusetts, USA: Benjamin-Cummings Pub. Co.

Cannell, M.G.R. 1982. *World Forest Biomass and Primary Production Data*. Academic Press, London, 391 pp.

Chikaraishi, Y., Naraoka, H. 2003. Compound-specific δD - $\delta^{13}C$ analyses of *n*-alkanes extracted from terrestrial and aquatic plants. *Phytochem.* 63, 361-371.

Chikaraishi, Y., Naraoka, H., Poulson, S. R. 2004a. Hydrogen and carbon isotopic fractionations of lipid biosynthesis among terrestrial (C3, C4, and CAM) and aquatic plants. *Phytochem.* 65, 1369-1381.

- Chikaraishi, Y., Naraoka, H., Poulson, S. R. 2004b. Carbon and hydrogen isotopic fractionation during lipid biosynthesis in a higher plant (*Cryptomeria japonica*). *Phytochem.* 65, 323-330.
- Craig, H. 1961. Isotopic variations in meteoric waters. *Science*, 133, 1702–1703.
- Crouch, E. M., Hellman-Clausen, C., Brinkhuis, H., Morgans, H. E. G., Rogers, K. M., Egger, H., Schmitz, B. 2001. Global dinoflagellate event associated with the late Paleocene thermal maximum. *Geology* 29, 315-318.
- Dawson, M. R., West, R. M., and Hutchinson, J. H. 1976. Paleogene terrestrial vertebrates: northernmost occurrence, Ellesmere Island, Canada. *Science*, 192, 781–782.
- Dawson, T.E., Mambelli, S., Plamboeck, A. H., Templer, P.H., Tu, K. P. 2002. Stable isotopes in plant ecology. *Ann. Rev. Ecol. Syst.* 33, 507-559.
- DeConto, R. M., Pollard, D. 2003. Rapid Cenozoic glaciation of Antarctica induced by declining atmospheric CO₂. *Nature* 421, 245-249.
- Dickens, G. R., Castillo, M. M., Walker, J. C. G. 1997. A blast of gas in the latest Paleocene: simulating first-order effects of massive dissociation of oceanic methane hydrate. *Geology* 25, 259-262.
- Dickens, G. R. 2001. The potential volume of oceanic methane hydrates with variable external conditions. *Org. Geochem.* 32, 1179-1193.
- Diester-Haass, L., Zahn, R. 1996. Eocene-Oligocene transition in the Southern Ocean: history of water mass circulation and biological productivity. *Geology* 24, 163-166.
- Eberle, J. J. and Storer, J. E. 1999. Northernmost record of brontotheres, Axel Heiberg Island, Canada – Implications for age of the Buchanan Lake Formation and brontothere paleobiology. *J. Paleontology* 73, 979-983.
- Ekart, D. D., Cerling, T. E., Montanez, I. P., Tabor, N. J. 1999. A 400 million year carbon isotope record of pedogenic carbonate: implications for paleoatmospheric carbon dioxide. *Am. J. Sci.* 299, 805-827.
- Elder, J. F., and Cairns, D. J. 1982. Production and decomposition of forest litter fall on the Apalachicola River flood plain, Florida. *U. S. Geol. Surv. Water Supply Pap.* 2196B, 42.
- Emanuel, K. 2001. A simple model of multiple climate regimes. *J. Geophys. Res.* 107, 10 pgs.
- Emanuel, K. Personal communication. 10 June 2005.

Farquhar, G.D., Hubick, K.T., Condon, A.G. & Richards, R.A. 1989. Carbon isotope fractionation and plant water use efficiency. In *Stable isotopes in ecological research* (ed. W. Rundel, J.R. Ehleringer & K.A. Nagy). 68, 21-40. Springer.

Farley, K. A., Montanari, A., Shoemaker, E. M., Shoemaker, C. S. 1998. Geochemical evidence for a comet shower in the late Eocene. *Science* 280, 1250-1253.

Farley, K. A., Eltgroth, S. F. 2003. An alternative age model for the Paleocene-Eocene thermal maximum using extraterrestrial ^3He . *Earth Plan. Sci. Letters* 208, 135-148.

Ficken, K. J., Li, B., Swain, D. L., Eglinton, G. 2000. An *n*-alkane proxy for the sedimentary input of submerged/floating freshwater aquatic macrophytes. *Org. Geochem.* 31, 745-749.

Flanagan, L. B., Brooks, J. R., Ehleringer, J. R. 1997. Photosynthesis and carbon isotope discrimination in boreal forest ecosystems: a comparison of functional characteristics in plants from three mature forest types. *J. Geophys. Res.* 102, D24, 28861-28869.

Foscolos, A. E., and McMillan, N. J. 1991. An incipient Tertiary soil profile formed on grey clay and biogenic phytolite (white layer), Axel Heiberg Island. In *Tertiary Fossil Forests of the Geodetic Hills, Axel Heiberg Island, Arctic Archipelago*, R. L. Christie and N. J. McMillan (eds.); Geological Survey of Canada, Bulletin 403, 201-208.

Francis, J. E. 1991. The dynamics of polar fossil forests: Tertiary fossil forests of Axel Heiberg Island, Canadian Arctic Archipelago. In *Tertiary Fossil Forests of the Geodetic Hills, Axel Heiberg Island, Arctic Archipelago*, R. L. Christie and N. J. McMillan (eds.); Geological Survey of Canada, Bulletin 403, 29-38.

Fricke, H. C., Clyde, W. C., O'Neil, J. R., Gingerich, P. D. 1998. Evidence for rapid climate change in North America during the latest Paleocene thermal maximum: oxygen isotope compositions of biogenic phosphate from the Bighorn Basin (Wyoming). *Earth Plan. Sci. Letters* 160, 193-208.

Global Network of Isotopes in Precipitation. Copyright 2001, International Atomic Energy Agency and the World Meteorological Organization.
<http://isohis.iaea.org/GNIP.asp> .

Grattan, D. W. 1991. The conservation of specimens from the Geodetic Hills fossil forest site, Canadian Arctic Archipelago. In *Tertiary Fossil Forests of the Geodetic Hills, Axel Heiberg Island, Arctic Archipelago*, R. L. Christie and N. J. McMillan (eds.); Geological Survey of Canada, Bulletin 403, 213-227.

Greenwood, D. R., and Wing, S. L. 1995. Eocene continental climates and latitudinal temperature gradients. *Geology* 23, 1044-1048.

Grocke, D.R. 2002. The carbon isotope composition of ancient CO₂ based on higher-plant organic matter. *Phil. Trans. R. Soc. Lond. A* 360, 633-658.

Hayes, J. M. 2001. Fractionation of the isotopes of carbon and hydrogen in biosynthetic processes. Presented at GSA, November 2001. <http://Nosams.who.edu/jmh/>.

Huber, M. 3. Straw Man 1: a preliminary view of the tropical Pacific from a global coupled climate model simulation of the early Paleogene. *Proc. Oc. Drill. Prog. Init. Rep.* 1999.

Irving, E. and Wynne, P. J. 1991. The paleolatitude of the Eocene fossil forests of Arctic Canada. In *Tertiary Fossil Forests of the Geodetic Hills, Axel Heiberg Island, Arctic Archipelago*, R. L. Christie and N. J. McMillan (eds.); Geological Survey of Canada, Bulletin 403, 209-212.

Ivany, L. C., Patterson, W. P., Lohmann, K. C. 2000. Cooler winters as a possible cause of mass extinctions at the Eocene/Oligocene boundary. *Nature* 407, 887, 890.

Jahren, A. H. and Sternberg, L. S. L. 2002. Eocene meridional weather patterns reflected in the oxygen isotopes of Arctic fossil wood. *GSA Today*, January 2002, 4-9.

Jahren, A. H. and Sternberg, L. S. L. 2003. Humidity estimate for the middle Eocene Arctic rainforest. *Geology* 31, 463-466.

Jahren, A. H., LePage, B. A., Werts, S. P. 2004. Methanogenesis in Eocene Arctic soils inferred from $\delta^{13}\text{C}$ of tree fossil carbonates. *Palaeo. Palaeo. Palaeo.* 214, 347-358.

Jiang, C., Alexander, R., Kagi, R. I., Murray, A. P. 1998. Polycyclic aromatic hydrocarbons in ancient sediments and their relationships to paleoclimate. *Org. Geochem.* 729, 1721-1735.

Katz, M. E., Pak, D. K., Dickens, G. R., Miller, K. G. 1999. The source and fate of massive carbon input during the latest Paleocene thermal maximum. *Science* 286, 1531-1533.

Keeling, C. D., Whorf, T. P. 1998. Atmospheric CO₂ concentrations-Mauna Loa Observatory, Hawaii 1958-1997, <http://cdiac.esd.ornl.gov/ftp/ndp001/maunaloa.co2>.

Kelly, E.F., Blecker, S. W., Yonker, C. M., Olson, C. G., Wohl, E.E., Todd, L. C. 1998. Stable isotope composition of soil organic matter and phytoliths as paleoenvironmental indicators. *Geoderma* 82, 59-81.

Kennett, J. P., Stott, L. D. 1991. Abrupt deep-sea warming, palaeoceanographic changes and benthic extinctions at the end of the Palaeocene. *Nature* 353, 225.

Kennett, J. P., Cannariato, K. G., Hendy, I. L., Behl, R. J. 2000. Carbon isotopic evidence for methane hydrate instability during Quaternary interstadials. *Nature* 288, 128-133.

Kent, D. V., Cramer, B. S., Lanci, L., Wang, D., Wright, J. D., Van der Voo, R. 2003. A case for a comet impact trigger for the Paleocene/Eocene thermal maximum and carbon isotope excursion. *Earth Plan. Sci. Lett.* 211, 13-26.

Khalil, M. A. K., Shearer, M. J. & Rasmussen, R. A. 2000. Methane sinks, distribution and trends. In *Atmospheric methane* (ed. M. A. K. Khalil) p. 86. Springer.

Kirk-Davidoff, D. B., Schrag, D. P., Anderson, J. G. 2002. On the feedback of stratospheric clouds on polar climate. *Geophys. Res. Lett.* 29, 51-55.

Kojima, S., Sweda, T., LePage, B., Basinger, J. F. A new method to estimate accumulation rates of lignites in the Eocene Buchanan Lake Formation, Canadian Arctic. *Paleo. Paleo. Paleo.* 141, 115-122.

Korty, R. Personal communication.

Kunst, L., and Samuels, A. L. 2003. Biosynthesis and secretion of plant cuticular wax. *Prog. Lip. Res.* 42, 51-80.

Kurtz, A. C., Kump, L. R., Arthur, M. A., Zachos, J. C., Paytan, 2003. A. Early Cenozoic decoupling of the global carbon and sulfur cycles. *Paleocean.* 18, 1090-1104.

Lear, C. H., Elderfield, H., and Wilson, P. A. 2000. Cenozoic deep-sea temperatures and global ice volumes from Mg/Ca in benthic foraminiferal calcite: *Science* 287, 269–272.

Leavitt, S. W., and Long, A. 1982. Evidence for $^{13}\text{C}/^{12}\text{C}$ fractionation between tree leaves and wood. *Nature* 298, 742-744.

LePage, B. A., and Basinger, J. F. 1991. Early Tertiary *Larix* from the Buchanan Lake Formation, Canadian Arctic Archipelago, and a consideration of the phytogeography of the genus. In *Tertiary Fossil Forests of the Geodetic Hills, Axel Heiberg Island, Arctic Archipelago*, R. L. Christie and N. J. McMillan (eds.); Geological Survey of Canada, Bulletin 403, 67-82.

LePage, B. A., Yang, H., Matsumoto, M. 2005. The evolution and biogeographic history of *Metasequoia*. In *The Geobiology and Ecology of Metasequoia*, ed. B. A. LePage, C. J. Williams and H. Yang. Springer.

Luo, Y., and Sternberg, L.S.L. 1992. Hydrogen and oxygen isotopic fractionation during heterotrophic cellulose synthesis. *Journal of Experimental Botany*, 43, 47–50.

MacIntyre, D. J. 1991. Pollen and spore flora of an Eocene forest, Eastern Axel Heiberg Island, N. W. T. In *Tertiary Fossil Forests of the Geodetic Hills, Axel Heiberg Island*,

- Arctic Archipelago*, R. L. Christie and N. J. McMillan (eds.); Geological Survey of Canada, Bulletin 403, 83-98.
- Marco, M., Ferrara, C., Da Pelo, S., Ibba, A. 2003. The Palaeocene-Middle Eocene deposits of Sardinia (Italy) and their palaeoclimatic significance. *C. R. Geosci.* 335, 227-238.
- Mendoza, L., Tapia, L., Wilkens, M., Urzua, A. 2002. Antibacterial activity of 13-epi-sclareol, a labdane type diterpene isolated from *Pseudognaphalium heterotrichium* and *P. cheiranthifolium* (Asteraceae). *Bol. Soc. Chil. Quím.*, 47, 091-098.
- Millar, A. A., Clemens, S., Zachgo, S., Giblin, E. M., Taylor, D. C., Kunst, L. 1999. *CUT1*, an *Arabidopsis* gene required for cuticular wax biosynthesis and pollen fertility, encodes a very-long-chain fatty acid condensing enzyme. *The Plant Cell* 11, 825-838.
- Murray, A. P. 1998. Factors controlling the abundance and carbon isotopic composition of land-plant derived compounds in crude oils. Dissertation, Curtin University of Technology.
- Nissenbaum, A., and Yakir, D. 1995. Stable isotope composition of amber. In *Amber, Resinite and Fossil Resins*, ed. Anderson and Crelling. American Chemical Society Symposium Series 617.
- Norris, R. D., and Rohl, U. 1999. Carbon cycling and chronology of climate warming through the Palaeocene-Eocene transition. *Nature* 401, 775-778.
- Onnerud, H., Zhang, L., Gellerstedt, G., Henriksson, G. 2002. Polymerization of monolignols by redox shuttle-mediated enzymatic oxidation: a new model in lignin biosynthesis I. *The Plant Cell* 14, 1953-1962.
- Ourisson, G., Albrecht, P., Rohmer, M. 1979. The hopanoids. Palaeochemistry and biochemistry of a group of natural products. *Pure and App. Chem*, 51, 709-729.
- Pearson, P. N., and Palmer, M. R. 2000. Atmospheric carbon dioxide concentrations over the past 60 million years. *Nature* 406, 695-699.
- Pearson, P. N., Ditchfield, P. W., Singano, J., Harcourt-Brown, K. G., Nicholas, C. J., Olsson, R. K., Shackleton, N. J., Hall, M. A. 2001. Warm tropical sea surface temperatures in the Late Cretaceous and Eocene epochs. *Nature* 413, 481-487.
- Ravizza, G., and Peucker-Ehrenbrink, B. 2003. The marine $^{187}\text{Os}/^{188}\text{Os}$ record of the Eocene-Oligocene transition: the interplay of weathering and glaciation. *Earth Plan. Sci. Letters* 210, 151-165.
- Reale, S., Di Tullio, A., Spreti, N., De Angelis, F. 2003. Mass spectrometry in the biosynthetic and structural investigation of lignins. *Mass. Spec. Rev.* 23, 87-126.
- Retallack, G. J. 2001. A 300-million-year record of atmospheric carbon dioxide from fossil plant cuticles. *Nature* 411, 287-290.
- Retallack, G. J. 2002. Carbon dioxide and climate over the past 300 Myr. *Phil. Trans. R. Soc. Lond. A* 360, 659-673.

- Richter, S. L. and LePage, B. A. 2005. A high-resolution palynological analysis, Axel Heiberg Island, Canadian High Arctic. In *The Geobiology and Ecology of Metasequoia*, ed. B. A. LePage, C. J. Williams and H. Yang. Springer.
- Ricketts, B. D. 1991. Sedimentation, Eureka tectonism and the fossil forest succession on eastern Axel Heiberg Island, Canadian Arctic Archipelago. In *Tertiary Fossil Forests of the Geodetic Hills, Axel Heiberg Island, Arctic Archipelago*, R. L. Christie and N. J. McMillan (eds.); Geological Survey of Canada, Bulletin 403, 1-27.
- Ritchie, J.C. 1987. *Postglacial Vegetation of Canada*. Cambridge University Press, Cambridge.
- Robert, C. and Kennett, J. P. 1997. Antarctic continental weathering changes during Eocene-Oligocene cryosphere expansion: clay mineral and oxygen isotope evidence. *Geology* 25, 587-590.
- Roden, J.S., and Ehleringer, J.R. 1999. Hydrogen and oxygen isotope ratios of tree-ring cellulose for riparian trees grown long-term under hydroponically controlled environments. *Oecologia*, 121, 467-477.
- Royer, D.L., Wing, S. L., Beerling, D. J., Jolley, D. W., Koch, P. L., Hickey, L. J., Berner, R. A. 2001. Paleobotanical evidence for near present-day levels of atmospheric CO₂ during part of the Tertiary. *Science* 292, 2310-2313.
- Royer, D. L., Osborne, C. P., Beerling, D. J. 2002. High CO₂ increases the freezing sensitivity of plants: Implications for paleoclimatic reconstructions from fossil floras. *Geology* 30, 963-966.
- Royer, D. L., Osborne, C. P., Beerling, D. J. 2003. Carbon loss by deciduous trees in a CO₂-rich ancient polar environment. *Nature* 424, 60-63.
- Sachse, D., Radke, J., Gleixner, G. 2004. Hydrogen isotope ratios of recent lacustrine sedimentary *n*-alkanes record modern climate variability. *Geochim. Cosmochim. Acta* 68, 4877-4889.
- Sachse, D. 2005b. Compound-specific hydrogen isotope ratios of sedimentary *n*-alkanes: a new paleoclimate proxy. Dissertation. Universitat Jena, Germany.
- Sarangi, S., Sarkar, A., Sarin, M. M., Bhattacharya, S. K., Ebihara, M., Ray, A. K. 2001. Growth rate and life span of Eocene-Oligocene *Nummulites* tests: inferences from Sr/Ca ratio. *Terra Nova*, 13, 264-269.
- Sarkar, A., Sarangi, S., Ebihara, M., Bhattacharya, S. K., Ray, A. K. 2003. Carbonate geochemistry across the Eocene/Oligocene boundary of Kutch, western India: implications to oceanic O₂-poor condition and foraminiferal extinction. *Chem. Geol.* 201, 281-293.

- Sauer, P. E., Eglinton, T. I., Hayes, J. M., Schimmelman, A., Sessions, A. L. 2001. Compound-specific D/H ratios of lipid biomarkers from sediments as a proxy for environmental and climatic conditions. *Geochim. Cosmochim. Acta* 65, 213-222.
- Savidge, R. A., Forster, H. 2001. Coniferyl alcohol metabolism in conifers – II. Coniferyl alcohol and dihydroconiferyl alcohol biosynthesis. *Phytochem.* 57, 1095-1103.
- Savin, S. M. 1977. The history of earth's surface temperature during the past 100 million years. *Annu. Rev. Earth Planet. Sci.* 5, 319-355.
- Schoell, M. 1984. Recent advances in petroleum isotope geochemistry. *Org. Geochem.* 6, 645-663.
- Schoenhut, K. 2005. Ultrastructural preservation in Middle Eocene *Metasequoia* leaf tissues from the Buchanan Lake Formation. In *The Geobiology and Ecology of Metasequoia*, ed. B. A. LePage, C. J. Williams and H. Yang. Springer.
- Schulz, H.-M., Sachsenhofer, R. F., Bechtel, A., Polesny, H., Wagner, L. 2002. The origin of hydrocarbon source rocks in the Austrian Molasse Basin (Eocene-Oligocene transition). *Mar. Pet. Geol.* 19, 683-709.
- Schulze, T., Michaelis, W. 1990. Structure and origin of terpenoid hydrocarbons in some German coals. *Org. Geochem.* 16, 1051-1058.
- Segall, M. P., Siron, D. L., Colquhoun, D. J. 2000. Depositional and diagenetic signatures of Late Eocene-Oligocene sediments, South Carolina. *Sed. Geol.* 134, 27-47.
- Sessions, A. L., Burgoyne, T. W., Schimmelman, A., Hayes, J. M. 1999. Fractionation of hydrogen isotopes in lipid biosynthesis. *Org. Geochem.* 30, 1193-1200.
- Sessions, A. L., Jahnke, L. L., Schimmelman, A., Hayes, J. M. 2002. Hydrogen isotope fractionation in lipids of the methane-oxidizing bacterium *Methylococcus capsulatus*. *Geochim. Cosmochim. Acta* 66, 3955-3969.
- Sewall, J. O. and Sloan, L. C. 2004. Less ice, less tilt, less chill: the influence of a seasonally ice-free Arctic ocean and reduced obliquity on early Paleogene climate. *Geology* 32, 477-480.
- Shackleton, N. J. & Boersma, A. 1981. The climate of the Eocene ocean. *J. Geol. Soc. Lond.* 138, 153-157.
- Sheldon, N. D., Retallack, G. J., Tanaka, S. 2002. Geochemical climofunctions from North American soils and application to paleosols across the Eocene-Oligocene boundary in Oregon. *J. Geol.* 110, 687-696.

- Sloan, L. C., Morrill, C. 1998. Orbital forcing and Eocene continental temperatures. *Palaeo. Palaeo. Palaeo.* 144, 21-35.
- Sloan, L. C., Huber, M., Crowley, T. J., Sewall, J. O., Baum, S. 2001. Effect of sea surface temperature configuration on model simulations of “equable” climate in the Early Eocene. *Palaeo. Palaeo. Palaeo.* 167, 321-335.
- Smith, J. W., Gould, K. W., Rigby, D. 1982. The stable isotope geochemistry of Australian coals. *Org. Geochem.* 3, 111-131.
- Spicer, R. A. & Chapman, J. L. 1990. Climate change and the evolution of high-latitude terrestrial vegetation and flora. *Trends Ecol. Evol.* 5, 279–284.
- Staccioli, G., McMillan, N. J., Bartolini, G. 2002. Chemical characterization of a 45 million year bark from Geodetic Hills fossil forest, Axel Heiberg Island, Canada. *Wood Sci. Tech.* 36, 419-427.
- Stankiewicz, B. A., Briggs, D. E. G., Evershed, R. P. 1997. Chemical composition of Paleozoic and Mesozoic fossil invertebrate cuticles as revealed by pyrolysis-gas chromatography/mass spectrometry. *Energy & Fuels* 11, 515-521.
- Stankiewicz, B. A., Poinar, H. N., Briggs, D. E. G., Evershed, R., Poinar Jr., P & G. O. 1998. Chemical preservation of plants and insects in natural resins. *Proceedings of the Royal Society of London B*265. 641–647.
- Stuiver, M. and Brazunias, T. F. 1987. Tree cellulose $^{13}\text{C}/^{12}\text{C}$ ratios and climatic change. *Nature* 328, 58-60.
- Tarduno, J. A., Brinkman, D. B., Renne, P. R., Cottrell, R. D., Scher, H., Castillo, P. 1998. Evidence for extreme climatic warmth from late Cretaceous Arctic vertebrates. *Science* 282, 2241-2244.
- Tarnocai, C., Kodama, H., Fox, C. 1991. Characteristics and possible origin of the white layers found in the fossil forest deposits, Axel Heiberg Island. In *Tertiary Fossil Forests of the Geodetic Hills, Axel Heiberg Island, Arctic Archipelago*, R. L. Christie and N. J. McMillan (eds.); Geological Survey of Canada, Bulletin 403, 189-200.
- Thomas, D. J., Zachos, J. C., Bralower, T. J., Thomas, E., Bohaty, S. 2002. Warming the fuel for the fire: evidence for the thermal dissociation of methane hydrate during the Paleocene-Eocene thermal maximum. *Geology* 30, 1067-1070.
- Thomas, D. J., Bralower, T. J., Jones, C. E. 2003. Neodymium isotopic reconstruction of late Paleocene-early Eocene thermohaline circulation. *Earth Plan. Sci. Letters* 209, 309-322.

Tripati, A. K., and Elderfield, H. 2004. Abrupt hydrographic changes in the equatorial Pacific and subtropical Atlantic from foraminiferal Mg/Ca indicate greenhouse origin for the thermal maximum at the Paleocene-Eocene boundary. *Geochem. Geophys. Geosys.* 5, no. 2.

Tuo, J., Wang, X., Chen, J., Simoneit, B. R. T. 2003. Aliphatic and diterpenoid hydrocarbons and their individual carbon isotope compositions in coals from the Liaohe Basin, China. *Org. Geochem.* 24, 1615-1625.

Upchurch, Jr., G. R., Otto-Bliesner, B. L., Scotese, C. 1998. Vegetation-atmosphere interactions and their role in global warming during the latest Cretaceous. *Phil. Trans. R. Soc. Lond. B* 353, 97-112.

Vann, D. R. 2005. Physiological ecology of *Metasequoia glyptostroboides* Hu et Cheng. In *The Geobiology and Ecology of Metasequoia*, ed. B. A. LePage, C. J. Williams and H. Yang. Springer.

Wade, B. S., Kroon, D. 2002. Middle Eocene regional climate instability: Evidence from the western North Atlantic. *Geology* 30, 1011-1014.

Weatherbase. 2005. Copyright Canty and Associates LLC. <http://www.weatherbase.com>.

White, J. W. C. 1988. Stable isotope ratios in plants: A review of current theory and some potential applications, in Runderl, P. W., et al., eds., *Stable isotopes in ecological research*: Berlin, Springer-Verlag, 142-162.

Widdel, F. and Rabus, R. 2001. Anaerobic biodegradation of saturated and aromatic hydrocarbons. *Curr. Opin. Biotech.* 12, 259-276.

Williams, C. J., Johnson, A. H., LePage, B. A., Vann, D. R., Taylor, K. D. 2003a. Reconstruction of Tertiary Metasequoia forests. I. Test of a method for biomass determination based on stem dimensions. *Paleobiology* 29, 256-270.

Williams, C. J., Johnson, A. H., LePage, B. A., Vann, D. R., Sweda, T. 2003b. Reconstruction of Tertiary Metasequoia forests. II. Structure, biomass, and productivity of Eocene floodplain forests in the Canadian Arctic. *Paleobiology* 29, 271-292.

Wing, S. L., Bown, T. M., Obradovich, J. D. 1991. Early Eocene biotic and climatic change in interior western North America. *Geology* 19, 1189-1192.

Wing, S.L., and Greenwood, D.R., 1993. Fossils and fossil climate: The case for equable continental interiors in the Eocene. *Royal Society of London Philosophical Transactions*, ser. B, 341, 243-252.

- Yang, H. 2004. Biomolecules from living and fossil *Metasequoia*: biological and geological applications. In *The Geobiology and Ecology of Metasequoia*, ed. B. A. LePage, C. J. Williams and H. Yang. Kluwer Academic Publishers.
- Yang, H., Huang, Y., Leng, Q., LePage, B. A., Williams, C. J. 2005. Biomolecular preservation of Tertiary *Metasequoia* fossil *Lagerstätten* revealed by comparative pyrolysis analysis. *Rev. Paleobot. Palyn.* 134, 237-256.
- Yapp, C. J. 2004. Fe(CO₃)OH in goethite from a mid-latitude North American Oxisol: Estimate of atmospheric CO₂ concentration in the early Eocene “climatic optimum.” *Geochim. Cosmochim. Acta* 68, 935-947.
- Zachos, J. C., Lohmann, K. C., Walker, J. C., Wise, S. W. 1993. Abrupt climate change and transient climates during the Paleogene: a marine perspective. *J. Geol.* 101, 191-213.
- Zachos, J. C., L. D. Stott, and K. C. Lohmann, 1994. Evolution of early Cenozoic marine temperatures. *Paleoceanography* 9, 353–387.
- Zachos, J., Pagani, M., Sloan, L., Thomas, E., Billups, K. 2001. Trends, rhythms and aberrations in global climate 65 Ma to present. *Science* 292, 686-693.
- Zachos, J. C., Wara, M. W., Bohaty, S. Delaney, M. L., Petrizzo, M. R., Brill, A., Bralower, T. J., Premoli-Silva, I. 2003. A transient rise in tropical sea surface temperature during the Paleocene-Eocene thermal maximum. *Science* 302, 1551-1554.
- Zavarin E., Cool L. 1991. Extraneous materials from wood. In: *Wood structure and composition* (Edited by M. Lewin and I. S. Goldstein) M. Dekker Inc. NewYork.

NORMALIZED ABUNDANCE

YOUNG	C15 (ug/g)	C16	C17	C18	C19	C20	C21	C22	C23	C24	C25	C26
K'												
J'												
29 I'							5.235820896	2.634825871	13.03084577	4.926368159	23.09154229	5.347263682
28 H' rich			#VALUE!	#VALUE!	#VALUE!	#VALUE!	#VALUE!	#VALUE!	#VALUE!	#VALUE!	#VALUE!	#VALUE!
27 H' lean				0.153846154	0.611538462	0.634615385	2.951923077	2.296153846	10.59807692	3.251923077	8.966346154	3.061538462
26 H' bulk							2.146788991	1.868501529	8.370030581	3.464831804	8.844036697	2.706422018
25 G'							6.042105263	4.174162679	18.33492823	5.879425837	16.00287081	4.776076555
24 F'	0.514044944	1.13670412	1.595505618	6.261235955	3.18071161		9.337078652	8.396067416	36.13857678	13.8417603	28.81273408	10.58801498
23 E'							1.164867517	1.217860648	5.565260059	1.921491658	5.784102061	2.17468106
22 D'							3.447416974	3.506457565	13.25369004	8.564575646	13.74907749	6.373616236
21 C'												
20 B'						0.325024925	0.75772682	0.502492522	1.880358923	0.778664008	2.210368893	0.998005982
A'												
1 A			0.012731481	0.024305556	0.072916667	0.060185185	0.197916667	0.210648148	0.844907407	0.467592593	1.061342593	0.458333333
2 B			0.004798464	0.013435701	0.051823417	0.040307102	0.134357006	0.163147793	0.508637236	0.259117083	0.547024952	0.239923225
3 C				0.010794897	0.033366045	0.045142296	0.514229637	0.138370952	1.992149166	0.190382728	0.996074583	0.170755643
4 D			0.358938547	0.381284916	0.842178771	0.75698324	3.818435754	2.417597765	55.95111732	4.421787709	70.50837989	9.874301676
5 E						0.021978022	0.040959041	0.057942058	0.042957043	0.023976024	0.012987013	
36 HAG99-065				0.213333333	0.656	0.732	0.904	0.9	1.084	0.852	1.125333333	0.714666667
37 HAG99-066				0.032731377	0.153498871	0.267494357	0.374717833	0.431151242	0.495485327	0.38261851	0.477426637	0.32731377
38 HAG99-067				0.274576271	0.751694915	1.077966102	1.322033898	1.330508475	1.894067797	1.307627119	1.509322034	0.929661017
6 G							4.265306122	2.946938776	8.206122449	6.93877551	16.95306122	9.93877551
7 (rec) H			0.00862069	0.034482759	0.077586207	0.135057471	0.181992337	0.266283525	0.1848659	0.272988506	0.151340996	
8 I								1.347027972	5.734265734	2.173951049	7.113636364	2.923076923
9 J	0.894865526	1.268948655	1.476772616	5.441320293			5.311735941	5.575794621	21.17237164	10.89242054	23.53422983	10.50366748
10 K				0.503441495	0.373647984	1.065880039	1.12979351	4.198623402	1.912487709	8.157325467	4.605703048	
11 L					0.698207171	0.349601594	1.528884462	6.28685259	2.457171315	7.410358566	2.591633466	
12 M			0.076076994	0.214482126	0.54995417	0.501374885	0.961503208	1.125572869	3.96700275	1.543538038	4.116406966	1.866177819
13 N			0.403525955	0.377081293	1.637610186		2.486777669	2.053868756	7.839373164	4.163565132	13.80019589	4.254652302
14 O1	0.626799557	1.121816168	1.543743079	3.109634551	2.372093023	5.15282392	5.970099668	22.6854928	9.236987818	21.5282392	10.28017719	
15 O2	0.18611379	0.401157184	0.720347155	1.574734812	0.272902604	2.289296046	2.477338476	2.904532305	10.34522662	4.444551591	10.04146577	5.025072324
16 P	0						1.076559546	1.185255198	5.512287335	2.224007561	10.1758034	3.831758034
17 Q							3.273563218	4.156321839	16.32183908	7.402298851	26.76321839	9.28045977
18 R	0.488349515	0.87184466	0.977669903	2.233980583			10.37475728	8.522330097	97.42427184	14.94854369	101.5466019	16.50776699
19 S						1.291505792	1.310810811	1.254826255	6.587837838	2.404440154	8.760617761	1.968146718
S1												
T												
U												

CONCENTRATION OF n-ALKANES IN EACH SAMPLE

OLD	C15	C16	C17	C18	C19	C20	C21	C22	C23	C24	C25	C26
36 HAG99-065				0.213333333	0.656	0.732	0.904	0.9	1.084	0.852	1.125333333	0.714666667
37 HAG99-066				0.032731377	0.153498871	0.267494357	0.374717833	0.431151242	0.495485327	0.38261851	0.477426637	0.32731377
38 HAG99-067				0.274576271	0.751694915	1.077966102	1.322033898	1.330508475	1.894067797	1.307627119	1.509322034	0.929661017
				0.520640981	1.561193787	2.077460458	2.600751731	2.661659716	3.473553124	2.542245629	3.112082004	1.971641453

C27	C28	C29	C30	C31	C32	C33	C34	C35	Paq	CPI
45.2159204	9.200995025	48.26865672	8.167164179	12.97512438					0.37	4.88
#VALUE!	#VALUE!	#VALUE!	#VALUE!	#VALUE!	#VALUE!					
11.24326923	3.781730769	15.79038462	3.423076923	7.138461538		1.958653846			0.46	3.57
8.5382263	2.697247706	10.91743119	2.458715596	9.287461774	1.529051988	2.844036697			0.46	3.46
14.87559809	5.827751196	36.70334928	5.877511962	15.19808612		13.66889952			0.40	4.55
35.20224719	14.79775281	50.32116105	13.62827715	37.28183521	4.580524345	17.61610487	8.088951311		0.43	2.80
6.559371933	2.52404318	7.665358194	1.746810599	3.631010795					0.50	3.17
23.72601476	10.98339483	42.60147601	13.36439114	25.66143911					0.28	2.86
2.822532403	1.185443669	2.619142572	0.648055833	2.574277168	0.300099701	2.017946162	0.473579262		0.44	2.86
1.997685185	0.829861111	4.171296296	0.915509259	4.074074074	0.527777778	1.509259259	0.28125		0.19	3.69
0.834932821	0.335892514	1.785028791	0.298464491	1.247600768	0.393474088	0.12571977	0.011516315		0.26	2.99
0.512266928	0.152109912	0.372914622	7.389597645	0.133464181	0.046123651	0.053974485			0.86	0.57
138.5418994	9.870111732	34.1075419	5.819832402	5.111731844	2.998603352				0.76	8.46
										0.93
1.112	0.642666667	1.294666667	0.414666667	0.605333333	0.085333333	0.268			0.54	1.55
0.474040632	0.304740406	0.490970655	0.176072235	0.266365688	0.066591422	0.124153499			0.56	1.44
1.202542373	0.747457627	1.315254237	0.494067797	0.686440678	0.143220339	0.366101695			0.63	1.43
29.41428571	17.12244898	42.36734694	14.03265306	42.23265306	9.795918367	30.40204082	2.806122449		0.23	2.73
0.232758621	0.11302682	0.197318008	0.063218391	0.101532567					0.64	1.59
12.59527972	4.414335664	19.54020979	3.79458042	9.612762238	0.890734266	3.590034965			0.31	3.74
32.66870416	15.49266504	75.10268949	18.81051345	58.88630807	7.885085575	19.93398533	5.446210269		0.25	3.16
20.34611603	6.342182891	34.00196657	7.528023599	5.877089479	1.573254671				0.24	3.16
6.901394422	3.69123506	16.05776892	4.354581673	14.55677291	2.079681275	11.35059761			0.31	3.62
4.276810266	2.242896425	6.066911091	1.943171402	3.781851512	0.752520623	129.4225481		0.959670027	0.45	15.13
16.60920666	5.747306562	32.54260529	7.658178257	29.72771792	11.99216454	18.19980411	4.362389814	14.47894221	0.26	3.39
27.00885936	16.1683278	58.13621262	14.05647841	43.37984496	6.223698782	25.28682171	15.39091916	29.64451827	0.30	2.90
12.96528447	7.222757956	20.9045323	6.198649952	15.27000964	2.942140791	14.11861138	6.442622951	10.85728062	0.36	2.49
14.51134216	4.549149338	26.74952741	3.134215501	11.36200378		3.896975425			0.29	4.91
65.38390805	22.30804598	129.8022989	21.03448276	60.13103448	5.64137931	9.852873563			0.18	4.46
143.5378641	26.24660194	142.4640777	23.18446602	47.26019417	4.661165049	7.325242718	6.415533981		0.51	5.42
7.907335907	2.489382239	12.81081081	2.141891892	8.6496139	7.833011583	2.604247104			0.42	2.51

CONCENTRATION OF n-ALKANES IN EACH SAMPLE
(CONTINUED)

C27	C28	C29	C30	C31	C32	C33	C34	C35
1.112	0.642666667	1.294666667	0.414666667	0.605333333	0.085333333	0.268		
0.474040632	0.304740406	0.490970655	0.176072235	0.266365688	0.066591422	0.124153499		
1.202542373	0.747457627	1.315254237	0.494067797	0.686440678	0.143220339	0.366101695		
2.788583005	1.6948647	3.100891559	1.084806698	1.5581397	0.295145094	0.758255194	0	0

	C23	C25	C27	C29	C31
H'	8.37	8.84	8.54	10.92	9.29
G'	18.33	16.00	14.88	36.70	15.20
F'	36.14	28.81	35.20	50.32	37.28
D'	13.25	13.75	23.73	42.60	25.66
A	0.84	1.06	2.00	4.17	4.07
B	0.51	0.55	0.83	1.79	1.25
C	1.99	1.00	0.51	0.37	0.13
D	55.95	70.51	138.54	34.11	5.11
G	8.21	16.95	29.41	42.37	42.23
I	5.73	7.11	12.60	19.54	9.61
J	21.17	23.53	32.67	75.10	58.89
K	4.20	8.16	20.35	34.00	5.88
L	6.29	7.41	6.90	16.06	14.56
M	3.97	4.12	4.28	6.07	3.78
O	10.35	10.04	12.97	20.90	15.27
P	5.51	10.18	14.51	26.75	11.36
Q	16.32	26.76	65.38	129.80	60.13
R	97.42	101.55	143.54	142.46	47.26
S	6.59	8.76	7.91	12.81	8.65

M	120.73		-329.2565
mixed	150	-363.682	-326.1765

LIGNITES

dD vs. SMOW (with updated A, B, C and G, and corrected for C16)						
height	C23	C25	C27	C29	avg for layer	stdev for layer
68.14	-258.8854397	-254.685961	-248.8743523	-247.86437	-252.577531	5.16922322
71.36	-276.6355	-274.863	-267.3005	-256.102	-268.72525	9.33845782
72.88	-272.7825	-272.3963294	-259.362	-260.27125	-266.20302	7.38539297
78.47	-272.0101587	-280.1718141	-279.0960211	-275.8579817	-276.783994	3.67286431
92	-285.074	-282.3	-268.8	-263.72	-274.9735	10.3352321
93.02	-274.27	-270.03	-272.73	-265.91	-270.735	3.66305428
95.4	-282.62	-280.76	-273.97	-268.68	-276.5075	6.40715941
97.1	-276.1985	-279.08	-280.86	-285.19	-280.332125	3.76529212
107.3	-277.56	-278.04	-279.05	-271.33	-276.495	3.49888077
113.08	-271.85	-265.782	-265.172	-271	-268.451	3.46053965
116.48	-274.1	-269.2	-259.1	-247.8	-262.55	11.6488912
119.2	-266.107	-270.5045	-269.1481628	-273.214	-269.743416	2.95533697
120.05	-267.0545	-272.155	-268.4699942	-266.60625	-268.571436	2.5176227
120.73	-268.5494689	-264.7849885	-259.6620058	-262.6163298	-263.903198	3.74206398
124.29	-265.0005	-262.166	-256.0845	-259.4515	-260.675625	3.80800351
126.67	-257.8641152	-263.5352736	-256.5965677	-258.4237322	-259.104922	3.05087298
128.37	-238.297	-259.398	-245.848	-266.555	-252.5245	12.7944954
129.05	-283.437	-280.1155	-279.859	-295.0275	-284.60975	7.13378736
139.59	-273.226	-263.324	-253.6	-262.095	-263.06125	8.0382434

Error bars	(from best series)*	(takes C16 error into account)		
	C23	C25	C27	C29
H'I	3.73	5.88	5.87	5.60
G'	0.57	4.80	4.79	1.32
F'	0.95	2.13	0.48	1.71
D'	9.19	4.18	5.31	7.89
A	6.81	6.59	5.85	4.89
B	4.80	7.39	5.96	4.62
C	2.99	4.23	6.54	4.01
D	n/a	2.29	3.21	1.47
G	n/a	6.68	7.98	10.19
I	3.89	2.08	4.20	3.20
J	2.92	1.87	5.14	3.84
K	2.16	0.20	1.13	0.35
L	0.40	0.69	1.48	3.09
M	2.40	1.73	5.09	6.27
O	0.23	0.56	0.79	1.18
P	4.13	3.89	5.21	4.63
Q	n/a	1.97	3.70	3.43
R	0.32	0.32	0.36	0.05
S	0.56	0.97	1.43	n/a

n=1
n=2
n=3
n=4
n=5

red=overloaded peaks

*best series="series" means subsequent measurements made on the same day.
 Where multiple series were available, best series was chosen based on
 1) smallest daily RMS
 2) smallest daily H3 factor
 3) smallest standard deviation of triplicates/duplicates
 4) best quality of calibration standards

Average errors reported in text incorporate RMS from all days analyses were made.

Sample	RT (GC-FID)	RT (GCMS)	M+ Ion (GCMS)	Identity	RT (Delta)	D/H	amp 2	corr D/H	Average D/H	Std. dev D/H	avg stdev
4aa (D-layer)											
D1	27.726			C23	1835.23	-273.593	1258	-266.9039205	-276.1985	5.186920249	3.4957777
D2					1835.44	-270.309					
D3					2298.16	-281.702					
D4					2322.41	-279.19					
D1	30.906			C25	2012.25	-270.167			-274.575	4.023414553	
D2					2012.46	-272.422					
D3					2621.7	-279.075					
D4					2650.75	-276.636					
D1	33.922			C27	2182.17	-272.918			-275.141	2.799240969	
D2					2182.38	-273.384					
D3					2948.78	-279.075					
D4					2988.7	-275.187					
D3	36.445			C29	3189.76	-271.143			-269.7475	1.973535026	
D4					3207.73	-268.352					
D4	37.625			C30	3299.07	-272.726			-272.726		
10aa (K-layer)											
D3	27.522			C23	2271.62	-267.634			-266.107	2.15950411	0.7445439
D4					2273.29	-264.58					
D3	30.676			C25	2595.99	-270.646			-270.5045	0.200111219	
D4					2596.2	-270.363					
D4	32.13			C26	2737.27	-266.191			-266.191		
D1	33.642			C27	2171.93	-270.679			-270.5245	1.127188981	
D2					2171.93	-268.886					
D3					2917.64	-271.235					
D4					2917.01	-271.298					
D1	36.395			C29	2328.26	-272.7			-273.214	0.351840873	
D2					2328.26	-273.3					
D3					3224.24	-273.492					
D4					3219.65	-273.364					
D3	37.591			C30	3326.65	-276.509			-276.8055	0.419314321	
D4					3314.11	-277.102					
D3	38.823			C31	3448.92	-274.672			-274.82	0.209303607	
D4					3435.33	-274.968					
11aa (L-layer)											
D1	27.529			C23	2285.62	-267.335			-267.0545	0.396686904	4.0563181
D2					2289.18	-266.774					
D1	30.663			C25	2602.89	-271.666			-272.155	0.691550432	
D2					2606.86	-272.644					
D1	33.568			C27	2898.62	-263.744			-264.788	1.476438959	
D2					2902.38	-265.832					
D2	34.925			C28	3034.89	-257.088			-257.088		
D1	37.56			C30	3310.56	-257.091			-267.484	14.69792155	
D2					3314.32	-277.877					
D1	38.893			C31	3468.35	-253.783			-253.802	0.026870058	
D2					3473.37	-253.821					
D1	43.78			C35	3914.15	-206.819			-201.835	7.048440395	
D2					3918.33	-196.851					
12aa (M-layer)											
D1	27.513			C23	1920.08	-257.977					
D2											

SD RAW DATA FOR UGNITES

D1	30.642	C25	2093.34	-253.88			
D2							
D1	33.55	C27	2254.27	-244.517			
D2							
D1	36.276	C29	2408.31	248.871			
D2							
D4			3156.53	-252.044			
D1	38.796	C31	2546.46	-245.389			
D2							
13aa (N-layer)							
SNA							
D1	40.888	isoprenoid	3593.96	-318.695	-319.0715	0.532451406	0.5324514
D2			3600.02	-319.448			
14aa (O-layer 1)							
D3	27.65	C23	2309.03	-261.472	-265.9385	6.316584876	7.167677
D4			2306.52	-270.405			
D3	29.183	C24	2449.48	-235.376	-247.385	16.98329067	
D4			2445.3	-259.394			
D3	30.776	C25	2624.41	-254.336	-260.3295	8.476088986	
D4			2621.28	-266.323			
D3	32.205	C26	2758.17	-244.729	-250.087	7.577356267	
D4			2753.16	-255.445			
D2	33.7	C27	2171.3	-257.568	-253.717	7.863740395	
D3			2932.27	-244.67			
D4			2928.09	-258.913			
D3	35.056	C28	3059.34	-231.883	-238.368	9.171174952	
D4			3051.19	-244.853			
D2	36.539	C29	2332.23	-263.512	-263.2915	0.311834091	
D1			2331.6	-263.071			
D2	39.031	C31	2471.63	-261.213	-261.6665	0.641345851	
D1			2471.01	-262.12			
15aa (O-layer 2)							
D1	27.608	C23	2273.71	-265.165	-265.0005	0.232638131	0.403758
D2			2274.76	-264.836			
D1	30.736	C25	2585.96	-262.559	-262.166	0.55578593	
D2			2587	-261.773			
D1	33.663	C27	2884.41	-255.528	-256.0845	0.787009847	
D2			2885.87	-256.641			
D1	43.903	C35	3897.64	-220.591	-220.563	0.03959798	
D2			3899.73	-220.535			
16aa (P-layer)							
D1	22.462	?	1646.38	-365.899	-366.3545	0.644174278	5.9142619
D2			1647.13	-366.81			
D1	27.578	C23	1930.1	-291.071	-291.3405	0.381130555	
D2			1931.7	-291.61			
D1	30.729	C25	2107.56	-303.015	-289.26975	16.92999203	
D2			2109.23	-304.771			
D3			2591.18	-273.427			
D4			2589.72	-275.866			
D1	32.162	C26	2182.8	-259.042	-258.973	0.097580736	
D2			2184.89	-258.904			
D1	33.667	C27	2276.43	-305.956	-284.92975	25.44637615	
D2			2278.73	-307.944			
D3			2892.77	-263.621			
D4			2890.89	-262.198			
D1	34.979	C28	2342.89	-255.582	-254.3225	1.781201982	
D2			2345.4	-253.063			
D3	36.429	C29	3184.53	-262.537	-262.136	0.567099639	
D4			3182.23	-261.735			
D3	38.911	C31	3428.65	-267.348	-266.311	1.466539464	

SD RAW DATA FOR UGNITES
(CONTINUED)

D4					3427.39	-265.274			
17aa (Q-layer)									
D2	36.531			C29	2325.54	-276.172	-277.844	2.364565076	2.3645651
D1					2326.59	-279.516			
18aa (R-layer)									
D1	27.841			C23	2326.17	-283.209	-283.437	0.322440692	0.5318857
D2					2324.92	-283.665			
D1	30.993			C25	2646.78	-279.892	-280.1155	0.316076731	
D2					2644.69	-280.339			
D1	32.23			C26	2755.87	-273.119	-273.119		
D1	33.989			C27	2962.37	-280.111	-279.859	0.356381818	
D2					2959.44	-279.607			
D1	35.118			C28	3056	-280.025	-279.07	1.350573952	
D2					3054.12	-278.115			
D1	39.097			C31	3465.22	-284.05	-283.828	0.313955411	
D2					3461.25	-283.606			
19aa (S-layer)									
D1	36.367	?	?	C29	3162.17	-256.558	-254.454	2.975505335	2.9755053
D2					3159.03	-252.35			
22aa (D'-layer)									
D1	27.615			C23	2285.21	-272.343	-272.459	0.164048773	0.729469
D2					2287.3	-272.575			
D1	29.181			C24	2437.36	-267.247	-268.1235	1.239558187	
D2					2439.66	-269			
D1	30.75			C25	2599.96	-271.925	-271.6225	0.427799603	
D2					2602.26	-271.32			
D1	33.705			C27	2909.91	-260.096	-260.14	0.062225397	
D2					2912.42	-260.184			
D1	35.031			C28	3034.68	-260.119	-259.0585	1.499773483	
D2					3037.81	-257.998			
D1	36.487			C29	3213.79	-262.959	-262.564	0.558614357	
D2					3216.93	-262.169			
D1	37.681			C30	3317.25	-263.482	-262.3355	1.621395849	
D2					3319.76	-261.189			
D1	38.988			C31	3460.41	-256.779	-256.9645	0.262336616	
D2					3462.92	-257.15			
24aa (F'-layer)									
D1	27.708	33.444	324	C23	2291.89	-273.456	-272.7825	0.952472834	1.5504495
D2					2296.07	-272.109			
D1	29.219	35.9	338	C24	2435.9	-260.563	-261.3275	1.081166268	
D2					2439.45	-262.092			
D1	30.819	38.475	352	C25	2600.8	-265.652	-267.1605	2.133341159	
D2					2606.23	-268.669			
D2	32.218	40.751	366	C26	2740.83	-253.655	-253.655		
D1	33.76	43.231	380	C27	2900.5	-259.701	-259.362	0.479418398	
D2					2906.77	-259.023			
D1	35.063	45.39	394	C28	3028.41	-255.079	-254.343	1.040861182	
D2					3035.1	-253.607			
D1	37.691	49.644	422	C30	3296.56	-265.25	-262.6935	3.615436972	
D2					3308.89	-260.137			
25aa (G'-layer)									
D3	27.638			C23	2282.07	-277.038	-276.6355	0.569220959	3.395951
D4					2294.82	-276.233			
D3	30.759			C25	2592.44	-278.255	-274.863	4.797012404	
D4					2605.6	-271.471			
D3	33.661			C27	2885.66	-270.687	-267.3005	4.789234229	
D4					2899.25	-263.914			
D1	36.46			C29	2326.17	-257.037	-256.102	1.322289681	

SD RAW DATA FOR UGENTILES
(CONTINUED)

D2			2325.54	-255.167			
D3	38.949		3433.66	-263.753		-259.8625	5.501997864
D4		C31	3448.5	-255.972			
27aa (H'-lean)							
D2	24.165		1733.45	-259.751		-275.192	21.83687162
D1		C21	1729.06	-290.633			24.991762
D2	25.878		1828.96	-242.553		-258.899	23.11673489
D1		C22	1823.11	-275.245			
D2	27.599		1938.27	-306.023		-293.92125	27.49159571
D1		C23	1931.79	-327.046			
D3			2283.95	-271.995			
D4			2275.38	-270.621			
D2	29.139		2013.71	-250.635		-267.9295	24.45811645
D1		C24	2008.7	-285.224			
D2	30.719		2110.9	-289.205		-287.82525	25.05088773
D1		C25	2104.42	-322.766			
D3			2593.9	-269.283			
D4			2585.54	-270.047			
D2	32.151		2181.75	-243.72		-266.33	31.97536865
D1		C26	2176.32	-288.94			
D2	33.642		2277.68	-292.736		-285.844	29.83383329
D1		C27	2270.58	-325.227			
D3			2893.6	-262.012			
D4			2883.78	-263.401			
D2	34.967		2342.05	-244.341		-265.7315	30.25073521
D1		C28	2335.78	-287.122			
D3		C29	3181.82	-258.317		-259.6835	1.932522833
D4			3169.9	-261.05			
D2	38.868		2567.77	-261.712		-265.22675	23.96234587
D1		C31	2561.5	-300.12			
D3			3422.17	-249.099			
D4			3416.73	-249.976			
D2	?39.723	?C32	2621.49	-248.552		-273.301	35.00037146
D1			2614.59	-298.05			

SD RAW DATA FOR UGNHTES
(CONTINUED)

RAW

	C23	C25	C27	C29
A (1)	-286.791 -280.128	-286.491 -279.962	-278.091 -276.569	-286.77 -278.087
avg	-283.4595	-283.2265	-277.33	-282.4285
stdev	4.711452483	4.61670017	1.076216521	6.1398082
B (2)	-261.819 -261.236	-258.439 -266.21	-265.955 -264.469	-268.275 -269.382
avg	-261.819	-258.439	-265.955	-268.275
stdev	0.412243253	5.4949268	1.050760677	0.7827672
C (3)	-298.738 -286.935	-291.047 -275.97	-278.287 -259.395	-268.021 -252.359
avg	-292.8365	-283.5085	-268.841	-260.19
stdev	8.345981338	10.6610489	13.35866131	11.074706
G (6)	-273.066	-281.422 -270.381 -263.624	-285.894 -275.739 -275.466 -273.682	-284.517 -275.654 -271.633 -272.887
avg	-273.066	-271.809	-277.69525	-276.17275
stdev		8.98451941	5.541424208	5.8109406
I (8)	-264.051 -270.44	-261.711 -265.35	-259.162 -265.684	-265.245 -270.216

	avg	-267.2455	-263.5305	-262.423	-267.7305
	stdev	4.517705225	2.57316158	4.611750427	3.5150278
J (9)		-268.587	-266.276	-257.629	-256.427
		-267.769	-263.736	-259.962	-257.047
	avg	-268.178	-265.006	-258.7955	-256.737
	stdev	0.578413347	1.79605122	1.649680121	0.4384062

SD RAW DATA FOR LIGNITES

G	71.30	-24.439	-24.139	-24.300	-24.3400000	-24.101	-24.607	-24.304	-24.7010000
F	72.88	-25.206	-25.939	-25.123	-25.42266667				
E	77.12	-24.579	-24.481	-24.814	-24.62466667				
D	78.47	-24.12	-22.491	-22.689	-23.1				
C	82.88	-24.564	-24.52	-24.678	-24.58733333				
B	85.25	-24.968	-23.691	-24.426	-24.36166667	-20.983	-21.101	-21.3	-21.128
A	92	-24.779	-24.435	-24.594	-24.60266667				
B	93.02	-23.238	-23.405	-23.845	-23.496				
C	95.4	-24.6	-24.39	-22.699	-23.89633333				
D	97.1	-25.15	-25.12	-25.949	-25.40633333				
E	99.82	-24.13	-27.032	-24.097	-25.08633333				
F	102.88								
G	107.3	-25.707	-25.723	-25.575	-25.66833333				
H	110.7	-24.479	-24.407	-24.463	-24.44966667				
I	113.08	-25.67	-26.569	-25.845	-26.028				
J	116.48	-24.382	-24.312	-24.642	-24.44533333				
K	119.2	-24.684	-24.84		-24.762				
L	120.05	-29.431	-23.933	-24.087	-25.817				
M	120.73	-23.795	-24.481	-47.769	-24.138	-22.554	-22.922	-22.657	-22.711
N	121.75	-23.444	-23.426		-23.435				
O	124.29	-24.331	-24.574	-29.518	-24.4525				
P	126.67	-25.878	-25.289	-47.737	-25.5835				
Q	128.37	-24.846	-25.058	-25.096	-25				
R	129.05	-25.323	-25.417	-25.572	-25.43733333				
S	139.59	-24.273	-24.068	-24.265	-24.202				

red=not used;outlier

WIL 019	-22.255	-22.189	-21.898	-22.114	0.189949993
WIL 038	-21.121	-21.029	-20.988	-21.046	0.068110205
WIL 006	-21.638	-21.411	-21.817	-21.622	0.203472357
WIL 044	-21.847	-21.886	-21.799	-21.844	0.043577517
paleosol 006	-23.124				
	-25.959				
	-25.525				
	-25.742				
	0.30688434				
paleosol 007	-24.954				
	-24.67				
	-24.018				
	-24.812				
	0.20081833				
paleosol 008	-26.882				
	-24.428				
	-24.884				
	-24.656				
	0.32244069				

Peak number	Start time	Ret time	Width	Amp2	Amp3	Bkgd 2	Bkgd 3	Area all	rD 3H2/2H2	d 3H2/2H2	d 2H/1H
16ab #1 coinj G											
8	1338	1343.2	13.6	284	60	685.5	66.1	1.194	-247.984	-303.558	-303.558
11	1650.7	1659.3	15	562	120	707.5	69.4	3.024	-199.744	-258.883	-258.883
21	1940.1	1946.6	17.6	378	84	726.5	73.7	2.219	-213.534	-271.654	-271.654
25	2188.6	2203.7	18.4	785	155	739.4	75	5.357	-204.219	-263.028	-263.028
28	2301.9	2311.7	14.2	356	77	762.9	80.3	1.892	-183.115	-243.482	-243.482
16ab #2 coinj G											
7	1338	1343	15.3	332	69	687	66.1	1.373	-247.409	-303.025	-303.025
14	1650.7	1659.3	15.5	624	130	713.9	70.4	3.403	-193.01	-252.646	-252.646
24	1940.1	1946.8	18.4	415	93	739.1	74.8	2.439	-199.991	-259.112	-259.112
31	2188.6	2204.1	18.6	855	168	748.1	76.5	5.96	-203.631	-262.483	-262.483
35	2299.4	2312	16.9	386	82	771.7	82.2	2.198	-197.943	-257.215	-257.215
P BULK ab	Peak	Trial 1	Amp 2	Trial 2	Amp 2	Average	St Dev				
	1	-303.558	284	-303.025	332	-303.2915	0.37688791				
	2	-258.883	562	-252.646	624	-255.7645	4.41022499				
	3	-271.654	378	-259.112	415	-265.383	8.86853325				
	4	-263.028	785	-262.483	855	-262.7555	0.3853732				
	5	-243.482	356	-257.215	386	-250.3485	9.71069743				
ab coinj G 0000											
6	1527.2	1533.9	19.9	545	131	335.1	90.8	2.212	-119.901	-184.94	-184.94
ab coinj G 0001											
6	1528.4	1534.7	18.4	599	145	337.1	91.4	2.416	-118.04	-183.217	-183.217
P BULK ab	Peak	Trial 1	Amp 2	Trial 2	Amp 2	Average	St Dev				
	1	-184.94	545	-183.217	599	58.9476667	420.93455				
230940 16ac #1											
9	2040.5	2054.3	22.4	218	46	682.5	65.4	1.662	-183.31	-243.663	-243.663
15	2276	2293.1	21.9	702	136	707.3	69.6	5.427	-223.663	-281.034	-281.034
21	2399.9	2413.7	24.7	425	82	699.6	68	3.282	-250.565	-305.949	-305.949
001355 16ac #2											
9	2037.1	2054.1	27.2	226	46	679.8	65.5	1.831	-222.331	-279.801	-279.801
15	2275.6	2292.7	21.9	721	140	704.3	69.6	5.534	-222.771	-280.208	-280.208
P BULK ac	Peak	Trial 1	Amp 2	Trial2	Amp 2	Average	St Dev				
	1	-243.663	218	-279.801	226	-101.821333	277.56216				
	2	-281.034	702	-280.208	721	46.9193333	567.316649				
	3	-305.949	425	-250.364		-43.771	406.917818				
11812 18ab #1											
17	2057.4	2065.5	16.1	557	119	731.6	77.7	4.022	-221.976	-279.472	-279.472

SD OF PEAKS

25	2188.6	2201	18.4	978	208	706.4	70.5	7.372	-223.641	-281.014	-281.014
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022229 18ab #2

16	2058	2066	15.7	524	114	739.5	78.4	3.829	-206.06	-264.732	-264.732
23	2189.7	2201	17.8	943	201	715.6	71.7	7.097	-215.229	-273.224	-273.224

R BULK ab	Peak	Trial 1	Amp 2	Trial 2	Amp 2	Average	St Dev	
		1	-279.472	557	-264.732	524	-272.102	10.422754
		2	-281.014	978	-273.224	943	-277.119	5.50836183

ab coinj G 0004	6	1528.2	1534.9	19.9	751	180	336.9	91.1	3.088	-109.072	-174.911	-174.911
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ab coinj G 0005	6	1528.8	1535.5	17.1	758	181	336.2	90.1	3.093	-83.749	-151.46	-151.46
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ab coinj G 0006	6	1528.6	1535.7	21.3	873	205	332.3	91.3	3.728	-126.746	-191.279	-191.279
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R BULK ab	Peak	Trial 1	Amp 2	Trial 2	Amp 2	Trial 3	Amp 2	Average	St Dev	
		1	-174.911	751	-151.46	758	-191.279	873	-172.55	20.0142182

ac coinj G 0006	6	1527.4	1534.7	18.2	704	170	329.5	90.4	2.967	-108.17	-174.076	-174.076
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ac coinj G 0007	6	1527.2	1534.7	19.2	717	173	327.6	90.6	3.004	-106.17	-172.224	-172.224
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R BULK ac	Peak	Trial 1	Amp 2	Trial 2	Amp 2	Average	St Dev	
		1	-174.076	704	-172.224	717	-173.15	1.30956176

ab coinj G 0001	7	1527	1535.3	18.2	582	129	700	63.2	2.357	-104.407	-170.591	-170.591
	9	2254.3	2269.1	27.6	1124	224	712.9	66	8.092	-220.554	-278.155	-278.155

ab coinj G 0002	7	1527.2	1534.9	17.3	668	147	698.8	63.2	2.779	-115.932	-181.265	-181.265
	11	2254.1	2269.1	27.4	1276	244	715.7	66.4	9.468	-219.102	-276.81	-276.81

183512 19ab #1	7	2188	2202.4	28.4	1140	227	702.1	68.9	8.125	-218.128	-275.908	-275.908
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195623 19ab #2	6	2188.2	2200.4	24	791	159	691.4	66.3	4.559	-201.865	-260.848	-260.848
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S BULK ab	Peak	Trial 1	Amp2	Trial 2	Amp 2	Trial 3	Amp 2	Trial 4	Amp 2	Average	St Dev	
		1	-170.591	582	-181.265	668				-175.928	7.54765778	
		2	-278.155	1124	-276.81	1276	-275.908	1140	-260.848	791	-272.93025	8.10757327

SD OF POLYCYCLES
(CONTINUED)

27ac #1											
10	1899.8	1914.9	24.5	556	114	281.4	97.2	3.237	-209.393	-267.819	-267.819
11	1924.3	1932	17.3	329	70	281.4	97.2	1.626	-238.199	-294.496	-294.496
20	2451.8	2480.2	32.4	1459	287	343	111	20.994	-255.7	-310.704	-310.704
21	2484.2	2494.4	22.2	848	164	343	111	6.678	-293.194	-345.427	-345.427

27ac #2											
9	1899.4	1911.7	22.4	485	100	266.4	94.6	2.684	-222.406	-279.87	-279.87
10	1921.8	1928.7	17.8	286	61	266.4	94.6	1.376	-248.127	-303.69	-303.69
16	2445.5	2469.3	28.6	1016	198	300.6	101.6	10.972	-249.489	-304.952	-304.952
17	2474.1	2482.9	28.2	527	105	300.6	101.6	3.636	-301.385	-353.013	-353.013

27ac #3											
9	1898.1	1912.1	23.6	530	109	266.6	94.2	3.015	-211.168	-269.463	-269.463
10	1921.8	1929.1	20.3	315	65	266.6	94.2	1.601	-248.564	-304.095	-304.095
16	2445.1	2469.5	29.1	1077	211	302.3	101.8	12.121	-249.194	-304.678	-304.678
17	2474.1	2483.3	26.5	568	112	302.3	101.8	3.961	-297.199	-349.136	-349.136

H' BULK ac	Peak	Trial 1	Amp2	Trial 2	Amp 2	Trial 3	Amp 2	Average	St dev	
	1	-267.819		556	-279.87	485	-269.463	530	-272.384	6.53496985
	2	-294.496		329	-303.69	286	-304.095	315	-300.760333	5.42884982
	3	-310.704		1459	-304.952	1016	-304.678	1077	-306.778	3.40277475
	4	-345.427		848	-353.013	527	-349.136	568	-349.192	3.79331003

SD OF POLYCYCLES
(CONTINUED)

Sample	M/Z	#C	#H	deg. unsat.	Base Peak	#C	#H	deg. unsat.	Identity of Compound	dD
16ab	284	21	32	6	255	19	27	6	tricyclic terpenoid with aromatized ring?	-336.60
	328	24	40	5	136	10	16	3	bicyclic with aromatized ring?	-279.75
	394	29	46	7	138	10	18	2	unknown dimer? (Stout 1995)	-297.38
	424	31	52	6	145	11	13	5	unknown dimer w/ two monoaromatic bicyclics? (Stout 1995)	-283.99
16ac	252	19	24	8	252	19	27	6	simonellite	-303.77
	342	25	42	5	342	25	42	5	bicyclic with aromatized ring?	-304.59
	324	24	36	7	324	24	36	7	sesterterpenoid with aromatized ring?	-311.09
18ab	406	30	46	8	57	4	9	0	dimeric cadenine? (Stout 1995)	-299.55
	440	32	56	5	367	27	43	6	17A(H)-bishomohopane	-295.72
18ac	432	32	48	9	55	4	7	1	full hopanoid with aromatized 6-mem-ring, 5-mem-ring?	-278.49
	324	24	36	7	324	24	36	7	sesterterpenoid with aromatized ring?	-305.16
	324	24	36	7	324	24	36	7	sesterterpenoid with aromatized ring?	-345.51
19ab	270	20	30	6	255	19	30	5	dehydroabietane	-198.19
	424	31	52	6	367	27	43	6	homohop-17(21)-ene, 17B(H)-homohop-29(31)-ene	-289.86
19ac	340	25	40	6	168	12	24	7	tricyclic with aromatized ring?	-256.85
25ab	440	32	56	5	367	27	43	6	B bishomohopane	n/a
25ac	324	24	36	7	324	24	36	7	sesterterpenoid with aromatized ring?	-323.28
	324	24	36	7	324	24	36	7	sesterterpenoid with aromatized ring?	-375.87

dD DATA		(ab listed first, then ac)								avg	stdev	
Layer	Height (m)	Peak 1	Peak 2	Peak 3	Peak 4	Peak 5	Peak 6	Peak 7	Peak 8			
G' (25)	71.36	-299.42138	-336.53039	-323.2768923	-375.86827					-311.09	-333.77	31.9886258
P (16)	126.67	-336.60	-279.75	-297.38	-283.99	-285.19	-303.77	-304.59			-300.30	18.4760999
R (18)	129.05	-299.55	-295.72	-278.49	-305.16	-345.51					-304.89	24.7981044
S (19)	139.59	-198.19	-289.86	-266.35							-251.46	47.6128432
ERRORS												
Layer	Height (m)											
G'	71.36	9.96	8.66	3.94	11.17	0.00	0.00	0.00			0	0
P	126.67	3.61	7.58	12.40	4.27	11.84	27.76	3.93			42.71	0
R	129.05	12.36	7.96	29.81	6.80	5.92	0.00	0.00			0	0
S	139.59	7.57	7.90	4.00	0	0	0	0			0	0

POLYCYCLIC MASS SPECTRA INFORMATION

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Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs. VSMOW
Duplicate 1											
1	19.4	20.5	23.4	5532	1002	33.2	25.3	105.576	-435.522	-477.237	-477.237
2	99.1	100.1	23.4	5508	998	33.3	25.4	105.161	-435.381	-477.106	-477.106
3	198.6	199.6	23.6	5533	992	33.4	25.3	105.198	-435.351	-477.078	-477.078
4	298.2	299.1	23.2	5540	986	33.4	25.3	104.052	-435.347	-477.075	-477.075
5	507.5	525.4	91.3	1544	435	36.3	26.2	32.7	-23.067	-95.262	-95.262
6*	1141.1	1178.6	119.5	4145	1213	41.1	27.5	113.312	0	-73.9	-73.9
7	2029.4	2042.3	46.8	72	19	36.7	26.4	1.383	-113.263	-178.793	-178.793
8	2236.5	2252.6	61.7	190	42	36	25.8	3.713	-173.891	-234.94	-234.94
9	2394.1	2408.5	53.5	104	24	36.7	26.2	2.02	-181.077	-241.596	-241.596
10	2546.7	2564.8	65.2	245	55	36.4	25.9	4.873	-182.673	-243.073	-243.073
11	2695.9	2710.7	56.2	105	25	37.3	25.8	2.079	-124.391	-189.098	-189.098
12	2839.5	2862.7	73.6	451	100	37.3	26	9.684	-181.206	-241.715	-241.715
13	2980.3	2997.5	63.3	200	45	39.1	26.7	3.94	-178.277	-239.003	-239.003
14	3115.4	3147.3	66	866	192	38.4	26.2	20.837	-192.207	-251.903	-251.903
15	3248.7	3266.3	58.1	229	51	43.3	27.6	4.454	-190.942	-250.731	-250.731
16	3363	3406.7	93.4	848	188	41.9	27.1	21.614	-191.294	-251.057	-251.057
17	3458.1	3477.3	43.3	59	13	57.7	30.7	1.018	-231.741	-288.515	-288.515
18	3502	3516	42	132	30	55.1	29.8	2.245	-157.627	-219.879	-219.879
19	3618.6	3640.8	74.4	403	90	50.7	29.1	8.262	-178.468	-239.179	-239.179
20	3726.3	3749.9	68.1	154	35	45	26.9	3.153	-117.136	-182.38	-182.38
21	3838.1	3862.5	59.4	63	16	41.8	26.8	1.393	-91.529	-158.665	-158.665
22*	3955.3	4018.7	126.2	2373	543	43.6	27.3	89.947	0	-244.1	-244.1
23	4995.5	4996.6	103.2	4299	752	37.9	27	409.978	-293.269	-465.782	-465.782
24	5115.1	5116.1	63.3	4236	748	33.5	25.4	244.764	-292.577	-465.259	-465.259
Duplicate 2											
1	19.2	20.3	23.2	4204	732	33.2	25.2	79.284	-432.852	-474.764	-474.764
2	98.9	99.9	23.2	4187	729	33.3	25.4	78.96	-432.985	-474.887	-474.887
3	198.6	199.4	23.2	4180	725	33.3	25.7	78.984	-433.244	-475.127	-475.127
4	298	298.9	23	4107	721	33.4	25.5	78.141	-432.97	-474.873	-474.873
5*	507	525.2	91.5	1612	453	36.8	26.8	34.125	-99.272	-99.272	-99.272
6*	1139.3	1178.3	120.4	4186	1226	41.7	28	116.792	0	-73.9	-73.9
7	2028.3	2041.9	47	79	20	36.7	26.2	1.487	-74.256	-142.668	-142.668
8	2235.3	2252.4	62.9	203	46	36	25.9	3.956	-171.897	-233.094	-233.094
9	2393.1	2408.1	56.2	113	26	36.7	26	2.186	-150.745	-213.505	-213.505
10	2545	2564.8	67.9	261	57	36.4	26.4	5.221	-200.066	-259.181	-259.181
11	2694.8	2710.5	57.1	114	27	37.3	26.1	2.237	-147.452	-210.456	-210.456
12	2837.2	2862.9	76.1	477	106	37.4	26.3	10.363	-186.127	-246.272	-246.272
13	2978.9	2997.7	65.2	214	48	39.3	27	4.209	-186.768	-246.866	-246.866
14	3111.4	3148.2	70.4	904	200	38.7	26.6	22.327	-195.221	-254.694	-254.694
15	3247.9	3266.5	59.8	244	55	43.9	27.5	4.756	-176.875	-237.704	-237.704
16	3362.8	3407.3	93.6	886	197	42.2	27.2	23.105	-190.743	-250.547	-250.547
17	3457.9	3477.6	43.3	62	13	59.4	31.6	1.067	-299.37	-351.147	-351.147
18	3502	3516.4	42.2	142	33	56.8	30.4	2.383	-167.197	-228.741	-228.741
19	3617.6	3641.4	75.7	424	95	52.5	29.5	8.734	-175.144	-236.101	-236.101
20	3725.2	3750.1	69.4	163	37	45.3	27.9	3.318	-187.609	-247.645	-247.645
21	3837.7	3862.5	62.1	67	17	41.8	26.9	1.507	-99.674	-166.208	-166.208
22*	3950.3	4018.7	131	2396	548	43.5	27.6	92.711	0	-244.1	-244.1
23	4995.5	4996.4	102.6	3272	555	38	27.2	308.879	-291.168	-464.194	-464.194
24	5114.9	5115.9	63.1	3231	552	33.5	25.6	184.71	-290.309	-463.545	-463.545
peak	start	ret	width	amp2	amp3	back 2	back 3	area all	rd 3h2/2h2	d 2h/1h	
1	19	37.7	22.4	1058	179	246.5	92.3	20.751	-441.483	-482.758	
2	99.1	117.5	23	1056	179	246.4	92.3	20.731	-441.373	-482.656	
3	198.6	212.6	22.2	1053	179	246.4	92.4	20.78	-442.171	-483.396	
4	298.2	299.3	22.6	1052	178	246.7	92.6	20.629	-442.104	-483.333	
5*	854.2	864.4	28.2	2205	528	249.9	92.8	11.283	0	-73.9	
6	1198	1203	14.8	123	30	252.5	93.6	0.513	-153.403	-215.967	
7	1302.9	1309	22.6	150	37	255.1	94.3	0.997	-166.877	-228.445	
8	1403	1411.8	41.4	426	102	257.2	94.5	5.244	-202.532	-261.465	
9	1473.4	1482.4	29.7	850	216	265.8	96.6	10.32	-136.78	-200.572	
10	1503.1	1509.6	37.6	543	129	265.8	96.6	7.079	-210.01	-268.391	
11	1593.6	1607	41	2176	496	263.3	95.7	28.172	-229.879	-286.791 C23	
12	1683.3	1694.2	42.6	1146	265	268.7	96.9	15.705	-224.975	-282.25	
13	1767.7	1785.3	57.6	2680	615	266.8	96.3	37.104	-229.555	-286.491 C25	
14	1853	1863.0	46.8	1075	252	277.9	97.1	15.921	-201.535	-260.541	
15	1952	1956.7	61	4812	1125	278.7	98.3	74.281	-220.485	-278.091 C27	
16	2012	2025.4	51	1820	432	301.4	103	30.902	-211.706	-269.961	
17	2083.1	2127	58.3	10707	2579	299.1	102.5	188.917	-229.857	-286.77 C29	
18	2141.4	2141.8	24.9	545	115	299.1	102.5	5.717	-299.058	-350.857	
19	2166.3	2184.7	46.2	3326	763	299.1	102.5	41.656	-221.476	-279.008	
20	2221.5	2276.8	61.7	9897	2337	335.1	109.9	190.527	-222.738	-280.178	
21	2283.1	2289.2	29.7	805	170	335.1	109.9	14.342	-286.683	-339.397	
22	2312.8	2328.1	21.3	3469	712	335.1	109.9	25.991	-216.309	-274.224	
23	2334.1	2344.6	18.2	799	162	335.1	109.9	6.099	-278.045	-331.397	
24	2352.3	2365.7	43.3	6247	1390	335.1	109.9	4.792	-272.025	-325.822	
25	2373.6	2404.3	13	50	10	335.1	109.9	0.415	-214.984	-272.997	
26	2416.9	2422.3	13	50	10	335.1	109.9	0.415	-313.162	-363.92	
27	2429.8	2452	36.6	1902	410	335.1	109.9	15.964	-251.53	-306.842	
28	2495.3	2502.4	11.7	237	52	312.8	105.1	1.073	-241.283	-297.352	
29	2507	2517.6	19.2	1799	383	312.8	105.1	10.905	-202.338	-261.285	
30	2526.2	2529.7	11.3	66	15	312.8	105.1	0.411	-273.539	-327.224	
31	2568.4	2574.7	17.6	245	59	313.6	105.6	1.335	-194.099	-253.655	
32	2629.2	2635.1	14.6	225	55	298.9	102.7	1.129	-161.445	-223.414	
33	2643.9	2651	14	70	17	298.9	102.1	0.5	-161.295	-223.275	
34	2657.9	2663.5	12.7	58	17	298.9	102.1	0.488	-176.12	-237.004	
35	2744.8	2759.4	24.2	115	29	300.4	103.2	0.834	-187.721	-247.749	
36	2769	2778.4	16.7	58	16	300.4	103.2	0.536	-214.187	-272.259	
37	2912	2921.6	22.2	79	19	296.7	102.7	0.638	-209.066	-267.516	
38	2934.2	2947.3	23.2	69	17	296.7	102.7	0.713	-252.873	-308.085	
39	3167.2	3183.5	28.4	60	15	283.6	98.4	0.884	-120.496	-185.491	
40	3198.7	3213.8	30.5	57	15	295.2	101.1	0.846	-160.616	-222.647	
41	3483.6	3484.9	32.4	1016	172	244.9	91.4	29.999	-440.924	-482.239	
42	3583.3	3594	31.8	1013	172	244	91.7	30.03	-441.861	-483.108	
1	19.4	20.5	22.2	1004	170	246.7	92	19.682	-442.842	-484.016	-484.016
2	97	106.2	25.7	1003	170	245	92.1	19.703	-443.796	-484.9	-484.9
3	198.6	209.4	21.9	999	169	245.7	92.4	19.706	-444.913	-485.934	-485.934
4	297.2	299.3	24.9	997	169	246.3	92.4	19.568	-443.981	-485.071	-485.071
5*	853.3	863	24.5	1986	485	248.7	92.9	9.796	0	-73.9	-73.9
6	1197.8	1202.4	12.7	50	13	248.7	92.2	0.237	-75.825	-144.121	-144.121
7	1302.9	1307.5	13.6	102	26	251.5	92.6	0.426	-58.809	-128.363	-128.363
8	1402.8	1409.5	17.1	544	122	251.1	92.9	2.204	-185.481	-245.674	-245.674
9	1473	1480.6	21.3	1030	233	259.3	95.4	4.483	-134.78	-198.719	-198.719
10	1498.9	1506.9	21.9	670	148	258.7	94.3	2.841	-193.533	-253.131	-253.131
11	1591.7	1604.7	28.4	2079	407	253.4	93.2	12.558	-222.984	-280.128 C23	-280.128 C23
1											

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Table with columns: peak, start, ret, width, amp2, amp3, back 2, back 3, area all, rd 3h2/2h2, d 2h/1h. Contains two main data blocks, one starting at peak 15 and another at peak 1. Many rows are highlighted in yellow.

Table with columns: peak, start, ret, width, amp2, amp3, back 2, back 3, area all, rd 3h2/2h2, d 2h/1h. Contains two main data blocks, one starting at peak 1 and another at peak 5. Many rows are highlighted in yellow.

laa CONT

22	2218.1	2227.1	16.7	434	87	291.3	101.3	2.182	-299.309	-351.09	-351.09
23	2234.8	2261	36.4	5931	1276	291.3	101.3	74.572	-220.406	-278.018	-278.018
24	2271.2	2282.3	19.4	952	187	291.3	101.3	6.316	-295.262	-347.342	-347.342
25	2290.6	2294	15.3	86	13	291.3	101.3	0.393	-414.661	-457.918	-457.918
26	2305.9	2317.6	18.4	1789	374	291.3	101.3	10.427	-219.032	-276.746	-276.746
27	2324.3	2331.4	20.5	400	83	291.3	101.3	2.82	-316.229	-366.76	-366.76
28	2344.8	2355.2	19	373	80	291.3	101.3	2.101	-302.063	-353.641	-353.641
29	2374	2392.4	36.2	3695	778	291.1	100.3	33.988	-213.008	-271.187	-271.187
30	2424.2	2439.9	19	753	151	313.3	105.6	4.538	-285.798	-320.054	-320.054
31	2443.2	2446.8	18	470	107	313.3	105.6	2.136	-254.536	-308.626	-308.626
32	2491.1	2496.5	13	96	22	292.6	100.9	0.448	-290.757	-315.387	-315.387
33	2504	2512.4	19	869	194	292.6	100.9	4.305	-204.96	-263.714	-263.714
34	2529	2531.2	13.2	51	12	292.6	100.9	0.39	-252.279	-307.536	-307.536
35	2567.8	2572.6	15	98	25	300.2	101.9	0.461	-97.343	-164.05	-164.05
36	2627.5	2633.2	15.5	95	24	296.3	102.6	0.478	-162.384	-224.284	-224.284
37	2643	2655.3	27	181	50	296.3	102.6	1.294	-142.248	-205.636	-205.636
38	3483.4	3487	32	959	162	243.1	91.8	28.319	-444.954	-485.972	-485.972
39	3583.1	3607.3	33.6	953	161	244.7	92.1	28.261	-444.959	-485.976	-485.976
1	19	28.8	24.9	944	159	247	92.7	18.543	-443.674	-484.787	-484.787
2	99.1	106.2	21.9	942	158	246.4	92.7	18.479	-444.237	-485.308	-485.308
3	198.6	204.2	22.6	941	159	245.2	91.6	18.568	-440.656	-481.992	-481.992
4	298.2	315	21.7	939	158	245.4	92.5	18.411	-443.418	-484.549	-484.549
5*	397.7	414.1	20.3	1689	416	249.2	93.1	8.292	0	-73.9	-73.9
6	497.2	513.5	19.4	83	17	249.6	92.8	0.285	-78.890	-146.965	-146.965
7	596.7	612.8	11.7	63	17	248.6	92.4	1.083	-192.085	-251.79	-251.79
8	696.2	712.1	16.7	134	32	250.6	92.6	0.605	-172.316	-233.482	-233.482
9	795.7	811.4	18.4	322	74	251.2	92.6	1.381	-186.448	-246.57	-246.57
10	895.2	910.8	16.7	124	30	252.8	93	0.58	-162.167	-224.083	-224.083
11	994.7	1010.2	21.3	613	137	250.6	92.7	2.785	-204.35	-263.148	-263.148
12	1094.2	1109.6	19.6	225	54	253.2	92.8	1.06	-192.598	-252.237	-252.237
13	1193.7	1208.9	20.3	1056	226	256.3	93	5.152	-191.412	-251.167	-251.167
14	1293.2	1308.1	16.5	148	33	268.6	95	0.665	-192.397	-252.078	-252.078
15	1392.7	1407.4	20.5	223	53	267.8	93.4	1.053	-177.184	-237.96	-237.96
16	1492.2	1506.8	23.8	889	198	261.8	94.2	4.384	-193.614	-253.206	-253.206
17	1591.7	1606.1	21.1	103	23	266.5	95.5	0.531	-283.835	-336.76	-336.76
18	1691.2	1705.4	15.3	113	23	262.2	94.2	0.555	-180.606	-241.243	-241.243
19	1790.7	1804.7	14.4	56	12	262.2	94.2	0.335	-292.063	-344.406	-344.406
20	1890.2	1904.1	19.2	338	81	265.3	93.6	1.637	-135.021	-198.943	-198.943
21	1989.7	2003.4	16.9	74	19	277.3	95.1	0.385	132.007	48.435	48.435
22	2089.2	2102.8	31.8	903	152	243.1	91.9	26.662	-445.395	-486.38	-486.38
23	2188.7	2202.1	33.4	899	153	243.9	91.7	26.663	-443.415	-484.546	-484.546

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peak	start	ret	width	amp2	amp3	back 2	back 3	area all	rd 3h2/2h2	d 2h/1h
1	19	34.9	22.2	883	149	246.2	92	17.331	-442.044	-483.277
2	99.1	111.6	22.2	882	149	246.7	92.4	17.302	-442.933	-484.1
3	198.6	203.1	21.7	881	148	245.8	92.6	17.361	-444.667	-485.707
4	298	311.8	21.7	877	147	247.3	92.5	17.192	-443.868	-484.967
5*	849.4	861.9	28.2	2543	609	247.9	92.9	13.83	0	-73.9
6	1194.9	1199.7	13.2	68	18	254.5	93.8	0.301	-76.543	-144.786
7	1299.6	1305	11.9	78	20	267.9	97.9	0.342	-157.772	-220.013
8	1400.5	1406.8	15	320	75	281.7	101.7	1.311	-172.833	-233.961
9	1497.1	1503.8	18	395	93	288	102.8	1.657	-153.056	-215.645
10	1590.3	1599.1	28	1102	233	285.8	102.5	5.316	-202.914	-261.819 C23
11	1679.9	1686.8	16.9	626	141	282.5	101.3	2.681	-192.118	-251.82
12	1765.8	1774.8	22.8	1196	244	274	98.5	5.64	-199.265	-258.439 C25
13	1848.4	1855.7	17.8	561	126	267.7	96.7	2.41	-186.049	-246.2
14	1927.6	1939.5	23.4	1648	339	260.5	93.1	9.144	-189.404	-249.307 C27
32+	1928.7	1939.5	22.4	1647	337	261.1	93.3	9.125	-207.38	-265.955 C27 alt
35+	1928.7	1939.5	22.4	1647	337	261.1	93.3	9.125	-207.38	-265.955 C27 alt
15	2006	2015	20.5	823	179	263.1	94.5	3.785	-187.406	-247.457
16	2082.9	2098.8	23.6	2942	601	263.5	94.8	22.772	-209.886	-268.275 C29
17	2106.5	2112.6	18	494	103	263.5	94.8	2.652	-274.743	-328.339
18	2155.6	2165.7	20.3	868	188	264.6	94.5	4.177	-197.498	-256.803
19	2212.9	2218.7	16.3	109	24	268.5	96	0.513	-292.22	-344.525
20	2229.2	2244.5	24.9	2639	528	268.5	96	18.735	-204.763	-263.531
21	2262.6	2270.8	20.7	317	68	284.9	98.6	1.471	-248.445	-303.985
22	2298.8	2306.9	16.7	493	112	268.9	95.6	2.266	-201.383	-260.401
23	2315.5	2322	17.3	303	65	268.9	95.6	1.584	-269.39	-323.382
24	2336.2	2345.4	17.8	108	24	271.2	95.4	0.655	-195.752	-255.186
25	2367.6	2378.4	21.3	1389	296	270.6	95.7	7.502	-189.15	-249.072
26	2417.3	2429.2	18.2	273	60	279.7	97.3	1.33	-214.754	-272.784
27	2435.5	2440.3	15.7	138	33	279.7	97.3	0.624	-168.051	-229.532
28	2498.4	2507.6	19.4	829	189	273.6	96.9	4.101	-176.639	-237.485
29	2621.3	2629.2	15.7	58	15	280.1	97.8	0.354	-99.228	-165.795
30	3483.2	3490.1	32	845	142	243.6	91.4	24.974	-442.523	-483.72
31	3582.3	3593.1	32.6	842	142	244.4	91.8	24.981	-443.223	-484.369

1	19	35.9	22.2	834	141	245.9	91.9	16.364	-442.43	-483.634
2	99.1	113.9	21.9	832	140	247.4	92.2	16.313	-442.707	-483.891
3	198.6	214.2	22.8	831	139	246.5	92.3	16.41	-442.966	-484.13
4	298.2	306.8	21.7	828	139	248.1	92.3	16.227	-442.569	-483.763
5*	851.3	863.6	28.4	2487	602	247.9	92.5	13.388	0	-73.9
6	1197.4	1201.5	13.2	84	22	257	93.4	0.355	34.953	-41.53
7	1272	1279.9	14	57	13	265.2	97	0.28	-181.993	-242.444
8	1301.9	1306.9	14.4	95	24	272.1	98.4	0.428	-86.813	-154.298
9	1402.6	1408.7	17.1	376	90	287.3	102.2	1.593	-138.544	-202.206
10	1499.4	1505.8	21.7	463	108	296.2	105	2.012	-165.763	-227.413
11	1592.8	1601.6	19.9	1279	258	291.6	104.2	6.167	-202.284	-261.236 C23
12	1681.8	1689.1	21.3	722	157	287.6	101.9	3.183	-184.204	-244.491
13	1767.5	1777.3	23	1327	271	277.6	99.7	6.693	-207.656	-266.21 C25
14	1850.1	1857.8	21.3	651	144	268.7	96.8	2.925	-186.54	-246.655
15	1929.9	1942.2	22.8	1848	373	262.5	95	10.774	-205.776	-264.489 C27
16	2008.3	2017.3	23.8	966	204	261.9	94.6	4.569	-201.932	-260.909
17	2083.9	2101.9	25.1	3316	678	262.2	94.4	27.017	-211.08	-269.382 C29
18	2109	2115.1	16.9	566	118	262.2	94.4	3.088	-271.585	-325.415
19	2158.1	2168.2	19.4	976	211	267.2	95.1	4.909	-200.194	-259.299
20	2215	2221	14.6	127	29	271.5	95.8	0.576	-220.435	-278.045
21	2231.5	2247.4	25.1	2889	592	271.1	95.5	22.056	-202.943	-261.846
22	2264.9	2273.3	20.5	365	78	286.3	98.8	1.723	-248.276	-303.829
23	2301.5	2309.4	16.3	579	132	267.9	95	2.734	-192.021	-251.731
24	2317.8	2324.3	19	350	74	267.9	95	1.876	-264.365	-318.728
25	2336.8	2347.7	20.3	132	30	267.9	95	0.854	-250.791	-306.158
26	2369	2381.1	22.2	1561	329	270	96	8.873	-197.544	-256.846
27	2425.2	2431.7	12.3	313	68	280.5	97.9	1.473	-239.728	-295.912
28	2437.6	2442.4	14.8	166	39	280.5	97.9	0.743	-213.964	-272.052
29	2500.3	2509.9	19.6	952	217	273.7	95.8	4.774	-162.291	-224.198
30	2625.9	2631.1	13.4	62	17	276.9	96.9	0.313	-52.729	-122.733
31	3482.6	3488.6	35.1	796	133	244.7	91.7	23.525	-443.77	-484.875
32	3583.1	3601.1	32	793	133	245.2	91.7	23.486	-443.177	-484.326

1	19.4	25.7	21.7	789	133	246.9	91.5	15.462	-443.167	-484.317
2	97	109.3	23.8	787	132	247.8	92.3	15.422	-446.292	-487.211
3	196	201.5	24.5	787	131	246.1	92.2	15.531	-447.116	-487.974
4	296.8	315.8	23	784	132	246.8	91.7	15.387	-443.975	-485.065
5*	855	864.2	21.7	1952	476	250.6	92.6	9.466	0	-73.9
6	1404.9	1409.7	13.2	84	21	260.5	95	0.363	-95.717	-162.543
7	1500.6	1506.5	14.6	103	25	260.4	94.9	0.453	-112.931	-178.486
8	1594.3	1600.3	16.9	335	79	260.7	95.2	1.426	-180.392	-240.961
9	1683.7	1689.1	13.2	162	42	259.5	91.6	0.693	29.191	-46.866
10	1768.3	1775.7	17.3	352	82	258.2	94.1	1.506	-182.925	-243.307
11	1851.9	1858	16.1	142	35	255.2	93.4	0.654	-181.872	-242.331
12	1930.7	1939.5	21.9	596	133	254	92.6	2.754	-193.806	-253.384
13	2009.5	2016	17.6	228	55	257.9	93.1	1.036	-163.064	-224.913
14	2085.8	2095.6	22.4	1192	253	256.8	92.1	6.29	-192.69	-252.35
15	2108.6	2113.8	12.5	115	26	274.6	96.3	0.514	-209.19	-267.631
16	2159.6	2166.1	16.7	230	56	260.4	93.6	1.088	-185.276	-245.484
17	2232.5	2241.3	22.6	964	211	262.7	93.5	4.861	-192.874	-252.52
18	2266	2271.8	15.3	77	18	270.9	95.3	0.37	-179.823	-240.434
19	2302.1	2308.4	15.7	118	28	261.9	94	0.593	-214.436	-272.49
20	2318.2	2322.8	13.4	77	17	269.4	95.3	0.354	-246.223	-301.927
21	2370.5	2377.8	19.2	394	93	265.3	94.3	1.872	-176.43	-237.292
22	2424.8	2430.5	13.4	64	14	271.8	95.9	0.304	-250.946	-306.301
23	2502.1	2508.4	17.6	189	47	269.2	95	0.89	-153.755	-216.292
24	3483.4	3499.5	31.8	753	126	245.7	91.6	22.19	-446.359	-487.273
25	3581.8	3608.2	34.9	749	125	245	92	22.212	-448.007	-488.799

peak	start	ret	width	amp2	amp3	back 2	back 3	area all	rd 3h2/2h2	d 2h/1h
1	19	34.9	22.2	883	149	246.2	92	17.331	-442.044	-483.277
2	99.1	111.6	22.2	882	149	246.7	92.4	17.302	-442.933	-484.1
3	198.6	203.1	21.7	881	148	245.8	92.6	17.361	-444.667	-485.707
4	298	311.8	21.7	877	147	247.3	92.5	17.192	-443.868	-484.967
5*	849.4	861.9	28.2	2543	609	247.9	92.9	13.83	0	-73.9
6	1194.9	1199.7	13.2	68	18	254.5	93.8	0.301	-76.543	-144.786
7	1299.6	1305	11.9	78	20	267.9	97.9	0.342	-157.772	-220.013
8	1400.5	1406.8	15	320	75	281.7	101.7	1.311	-172.833	-233.961
9	1497.1	1503.8	18	395	93	288	102.8	1.657	-153.056	-215.645
10	1590.3	1599.1	28	1102	233	285.8	102.5	5.316	-202.914	-261.819
11	1679.9	1686.8	16.9	626	141	282.5	101.3	2.681	-192.118	-251.82

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12	1765.8	1774.8	22.8	1196	244	274	98.5	5.64	-199.265	-258.439	-258.439
13	1848.4	1855.7	17.8	561	126	267.7	96.7	2.41	-186.049	-246.2	-246.2
14	1927.6	1939.5	23.4	1648	339	260.5	93.1	9.144	-189.404	-249.307	-249.307
32+	1928.7	1939.5	22.4	1648	339	260.5	93.1	9.14	-189.914	-249.78	-249.78
35+	1928.7	1939.5	22.4	1647	337	261.1	95.3	9.125	-207.38	-265.955	-265.955
15	2006	2015	20.5	823	179	263.1	94.5	3.785	-187.406	-247.457	-247.457
16	2082.9	2098.8	23.6	2942	601	263.5	94.8	22.772	-209.886	-268.275	-268.275
17	2106.5	2112.6	16	494	103	263.5	94.8	2.652	-274.743	-328.339	-328.339
18	2155.6	2185.7	20.3	868	188	264.6	94.5	4.177	-197.498	-256.803	-256.803
19	2212.9	2218.7	16.3	109	24	268.5	96	0.513	-292.22	-344.525	-344.525
20	2229.2	2244.5	24.9	2639	528	268.5	96	18.735	-204.763	-263.531	-263.531
21	2262.6	2270.8	20.7	317	68	284.9	96.6	1.471	-248.445	-303.985	-303.985
22	2298.8	2306.9	16.7	493	112	268.9	95.6	2.266	-201.383	-260.401	-260.401
23	2315.5	2322	17.3	303	65	268.9	95.6	1.584	-269.39	-323.382	-323.382
24	2336.2	2345.4	17.6	108	24	271.2	95.4	0.655	-195.752	-255.186	-255.186
25	2367.6	2378.4	21.3	1389	296	270.6	95.7	7.502	-189.15	-249.072	-249.072
26	2417.3	2429.2	18.2	273	60	279.7	97.3	1.33	-214.754	-272.784	-272.784
27	2435.5	2440.3	15.7	138	33	279.7	97.3	0.624	-168.051	-229.532	-229.532
28	2498.4	2507.6	19.4	829	189	273.6	96.9	4.101	-176.639	-237.485	-237.485
29	2621.3	2629.2	15.7	58	15	280.1	97.8	0.354	-99.228	-165.795	-165.795
30	3483.2	3490.1	32	845	142	243.6	91.4	24.974	-442.523	-483.72	-483.72
31	3582.3	3593.1	32.6	842	142	244.4	91.8	24.981	-443.223	-484.369	-484.369
1	19	35.9	22.2	834	141	245.9	91.9	16.364	-442.43	-483.634	-483.634
2	99.1	113.9	21.9	832	140	247.4	92.2	16.313	-442.707	-483.891	-483.891
3	198.6	214.2	22.8	831	139	246.5	92.3	16.41	-442.966	-484.13	-484.13
4	298.2	306.8	21.7	828	139	248.1	92.3	16.227	-442.569	-483.763	-483.763
5*	851.3	863.6	28.4	2487	602	247.9	92.5	13.388	0	-73.9	-73.9
6	1197.4	1201.5	13.2	84	22	257	93.4	0.355	34.953	-41.53	-41.53
7	1272	1279.9	14	57	13	265.2	97	0.26	-181.993	-242.444	-242.444
8	1301.9	1306.9	14.4	95	24	272.1	98.4	0.428	-86.813	-154.298	-154.298
9	1402.6	1408.7	17.1	376	90	287.3	102.2	1.593	-138.544	-202.206	-202.206
10	1499.4	1505.8	21.7	463	108	296.2	105	2.012	-165.763	-227.413	-227.413
11	1592.8	1601.6	19.9	1279	256	291.6	104.2	6.167	-202.284	-261.236	-261.236
12	1681.8	1689.1	21.3	722	157	287.6	101.9	3.183	-184.204	-244.491	-244.491
13	1767.5	1777.3	23	1327	271	277.6	99.7	6.693	-207.656	-266.21	-266.21
14	1850.1	1857.8	21.3	651	144	268.7	96.8	2.925	-186.54	-246.655	-246.655
15	1929.9	1942.2	22.8	1848	373	262.5	95	10.774	-205.776	-264.469	-264.469
16	2008.3	2017.3	23.8	966	204	261.9	94.6	4.569	-201.932	-260.909	-260.909
17	2083.9	2101.9	25.1	3318	678	262.2	94.4	27.017	-211.08	-269.382	-269.382
18	2109	2115.1	16.9	566	118	262.2	94.4	3.088	-271.585	-325.415	-325.415
19	2158.1	2168.2	19.4	976	211	267.2	95.1	4.909	-200.194	-259.299	-259.299
20	2215	2221	14.6	127	29	271.5	95.8	0.576	-220.435	-278.045	-278.045
21	2231.5	2247.4	25.1	2889	592	271.1	95.5	22.056	-202.943	-261.846	-261.846
22	2264.9	2273.3	20.5	365	78	286.3	98.8	1.723	-248.276	-303.829	-303.829
23	2301.5	2309.4	16.3	579	132	267.9	95	2.734	-192.021	-251.731	-251.731
24	2317.8	2324.3	19	350	74	267.9	95	1.876	-264.365	-318.728	-318.728
25	2336.8	2347.7	20.3	132	30	267.9	95	0.854	-250.791	-306.158	-306.158
26	2389	2381.1	22.2	1561	329	270	96	8.873	-197.544	-256.846	-256.846
27	2425.2	2431.7	12.3	313	68	280.5	97.9	1.473	-239.728	-295.912	-295.912
28	2437.6	2442.4	14.8	166	39	280.5	97.9	0.743	-213.964	-272.052	-272.052
29	2500.3	2509.9	19.6	952	217	273.7	95.8	4.774	-162.291	-224.196	-224.196
30	2825.9	2831.1	13.4	82	17	278.9	96.9	0.313	-52.729	-122.733	-122.733
31	3482.6	3488.6	35.1	796	133	244.7	91.7	23.525	-443.77	-484.875	-484.875
32	3583.1	3601.1	32	793	133	245.2	91.7	23.486	-443.177	-484.326	-484.326
1	19.4	25.7	21.7	789	133	246.9	91.5	15.462	-443.167	-484.317	-484.317
2	97	109.3	23.8	787	132	247.8	92.3	15.422	-446.262	-487.211	-487.211
3	196	201.5	24.5	787	131	246.1	92.2	15.531	-447.116	-487.974	-487.974
4	296.8	315.8	23	784	132	246.8	91.7	15.387	-443.975	-485.065	-485.065
5*	855	864.2	21.7	1952	476	250.6	92.6	9.466	0	-73.9	-73.9
6	1404.9	1409.7	13.2	84	21	260.5	95	0.363	-95.717	-162.543	-162.543
7	1500.6	1506.5	14.6	103	25	260.4	94.9	0.453	-112.931	-178.486	-178.486
8	1594.3	1600.3	16.9	335	79	260.7	95.2	1.426	-180.392	-240.961	-240.961
9	1883.7	1889.1	13.2	162	42	259.5	91.6	0.893	29.191	-46.866	-46.866
10	1788.3	1775.7	17.3	352	82	258.2	94.1	1.506	-182.925	-243.307	-243.307
11	1851.9	1858	16.1	142	35	255.2	93.4	0.654	-181.872	-242.331	-242.331
12	1930.7	1939.5	21.9	596	133	254	92.6	2.754	-193.806	-253.384	-253.384
13	2009.5	2016	17.6	228	55	257.9	93.1	1.036	-183.064	-224.913	-224.913
14	2085.8	2095.6	22.4	1192	253	256.8	92.1	6.29	-192.69	-252.35	-252.35
15	2108.8	2113.8	12.5	115	26	274.6	96.3	0.514	-209.19	-267.631	-267.631
16	2159.8	2186.1	16.7	230	56	260.4	93.6	1.098	-185.276	-245.484	-245.484
17	2232.5	2241.3	22.6	964	211	262.7	93.5	4.861	-192.874	-252.52	-252.52
18	2296	2271.8	15.3	77	18	270.9	95.3	0.37	-179.823	-240.434	-240.434
19	2302.1	2308.4	15.7	118	26	261.9	94	0.593	-214.436	-272.49	-272.49
20	2318.2	2322.8	13.4	77	17	269.4	95.3	0.354	-246.223	-301.927	-301.927
21	2370.5	2377.8	19.2	394	93	265.3	94.3	1.872	-178.43	-237.292	-237.292
22	2424.8	2430.5	13.4	64	14	271.8	95.9	0.304	-250.946	-306.301	-306.301
23	2502.1	2508.4	17.6	189	47	269.2	95	0.89	-153.755	-216.292	-216.292
24	3483.4	3499.5	31.8	753	126	245.7	91.6	22.19	-446.359	-487.273	-487.273
25	3581.8	3608.2	34.9	749	125	245	92	22.212	-448.007	-488.799	-488.799

peak	start	ret	width	amp2	amp3	back 2	back 3	area all	rd 3h2/2h2	d 2h/1h		
5*	1	19.4	25.5	21.7	742	124	248.1	92.4	14.55	-446.486	-487.391	-487.391
	2	98.6	116.6	22.2	742	124	247.1	92.1	14.541	-446.746	-487.631	-487.631
	3	198.6	204.8	21.7	740	124	246.7	91.6	14.584	-444.656	-485.696	-485.696
	4	298	309.1	21.7	737	123	246.7	92.5	14.425	-446.624	-487.518	-487.518
	5	853.8	864.4	23.8	2518	613	249.8	92.3	13.604	0	-73.9	-73.9
	6	1195.9	1202.6	14.4	159	41	254.9	94.1	0.624	-138.288	-201.969	-201.969
	7	1302.5	1308.3	16.3	331	82	260.8	95	1.334	-116.303	-181.608	-181.608
	8	1402.4	1417.2	30.5	2867	548	262.5	95.3	18.863	-223.379	-280.771	-280.771
	9	1499.6	1509	24	1103	236	268.4	96.4	5.22	-177.603	-238.378	-238.378
	10	1530.1	1535.9	20.3	172	38	272.9	97.3	0.982	-228.04	-285.087	-285.087
	11	1593.6	1619.1	35.7	6334	1330	272.2	97.7	76.35	-242.779	-298.738	-298.738
	12	1629.4	1637.7	15.9	253	57	272.2	97.7	1.756	-271.947	-325.751	-325.751
	13	1645.2	1649.4	9.6	102	21	272.2	97.7	0.63	-289.706	-342.197	-342.197
	14	1657.6	1662.6	16.1	103	23	309	105.1	0.511	-210.148	-268.518	-268.518
	15	1683.5	1693.7	24.9	1735	365	282.5	99.1	8.716	-206.741	-265.363	-265.363
	16	1769.2	1789	33.2	4304	856	274.5	97.8	38.898	-234.475	-291.047	-291.047
	17	1802.4	1808.5	10.2	106	24	274.5	97.8	0.614	-266.174	-320.404	-320.404
	18	1853.2	1862.4	20.5	1340	280	279.1	98.4	6.645	-196.214	-255.613	-255.613
	19	1932.4	1947.7	25.5	2841	570	275.4	97.8	20.767	-220.696	-278.287	-278.287
	20	2009.5	2020.4	24	1265	266	280	98.9	6.6	-201.775	-260.764	-260.764
	21	2081.8	2100.7	26.6	2449	500	280	98.7	17.314	-209.611	-268.021	-268.021
	22	2110.5	2117.8	16.5	564	117	280	98.7	3.063	-263.51	-317.936	-317.936
	23	2190	2169.8	16.3	1028	221	287.5	99.9	5.004	-191.654	-251.391	-251.391
	24	2176.3	2185.1	18.2	181	40	287.5	99.9	1.393	-270.832	-324.717	-324.717
	25	2218.1	2222.5	12.3	94	21	324.9	108.3	0.226	-319.098	-369.416	-369.416
	26	2230.4	2243.2	20.9	1419	298	324.9	108.3	7.133	-199.26	-258.435	-258.435
	27	2263.9	2275	22.8	442	93	305.9	103.7	2.203	-246.362	-302.056	-302.056
	28	2301.9	2309.4	16.9	339	81	284.2	98.6	1.710	-179.201	-239.858	-239.858
	29	2318.9	2324.9	17.3	355	77	284.2	98.6	1.835	-237.519	-293.867	-293.867
	30	2339.5	2348.1	17.1	183	42	292.7	100.5	1.022	-229.987	-286.891	-286.891
	31	2369	2378.8	21.3	702	163	291.4	100.6	3.36	-176.248	-237.121	-237.121
	32	2419.8	2433	19.2	502	107	298.6	101.9	2.531	-232.224	-288.962	-288.962
	33	2439	2442.8	11.7	90	22	298.6	101.9	0.394	-233.528	-290.17	-290.17
	34	2497.8	2508.4	20.9	295	74	294.5	101.1	1.339	-153.315	-215.885	-215.885
	35	3483.2	3487.6	32	708	118	247.3	92.2	20.896	-448.1	-488.886	-488.886
	36	3582.9	3610.9	32.2	705	118	247.5	91.8	20.915	-445.762	-486.72	-486.72
5*	1	19.4	26.5	21.7	700	118	250.2	91.5	13.708	-439.115	-480.564	-480.564
	2	99.1	106	21.7	698	117	250.3	92.5	13.676	-443.822	-484.924	-484.924
	3	198.6	201.3	23.8	697	117	249.2	92.4	13.745	-443.504	-484.629	-484.629
	4	298.2	304.9	21.7	696	116	249.5	92.4	13.63	-443.705	-484.815	-484.815
	5	852.3	863	24.9	2356	560	250.3	92.5	12.126	0	-73.9	-73.9
	6	1301.9	1306.5	11.9	81	21	252.5	93	0.336	-123.728	-188.484	-188.484
	7	1402.4	1410.5	19.9	1112	224	254.6	92.9	4.938	-202.166	-261.126	-261.126
	8	1497.9	1505	16.3	331	78	256.7	93.6	1.339	-158.211	-220.419	-220.419
	9	1591.3	1607	28.4	3009	576	257.3	93.6	20.993	-230.034	-286.935	-286.935
	10	1626	1632.5	15.3	52	13	272.7	96.3	0.257	-130.371	-194.636	-194.636
	11	1680.4	1688.1	23.2	549	125	263.1	93.8	2.338	-163.516	-225.332	-225.332
	12	1767.1	1779	23.6	1896	363	260.6	93.7	10.525	-218.195	-275.97	-275.97
	13	1850.5	1856.8	19	425	97	261.7	94.2	1.772	-180.846	-241.382	-241.382
	14	1928.9	1939.5	22.4	1166	240	260.9	93.2	5.705	-200.297	-256.395	-256.395
	15	2007.4	2014.6	18.6	394	92	262.7	94.1	1.821	-173.942	-234.988	-234.988
	16	2083.5	2092.5	22.2	947	204	264.2	94.4	4.669	-192.7	-252.359	-252.359
	17	2105.9	2111.9	16.9	152	34	273.1	96.1	0.655	-226.977	-284.104	-284.104
	18	2157.7	2164.2	14.4	298	70	266.9	94.4	1.324	-153.505	-216.061	-216.061
	19	2229.6	2236.9	17.6	429	99	267.4	95	2.101	-193.447	-253.051	-253.051
	20	2259.7	2269.5	17.6	115	25	273.2	95.8	0.565	-193.57	-253.165	-253.165
	21	2298.8	2305.9	16.5	87	22	266	94.5	0.461	-180.514	-241.074	-241.074
	22	2315.3	2320.3	13.2	95	22	266	94.5	0.488	-223.82	-281.18	-281.18
	23	2368.6	2374.7	15.5	191	47	270.7	95.2	0.895	-139.687	-203.264	-203.264
	24	2422.3	2428.2	14.4	130	30	273.2	95.8	0.641	-222.266	-279.74	-279.74
	25	2500.5	2505.9	16.9	80	20	270.4	95.4	0.41	-162.536	-224.424	-224.424
	26	3483.4	3488.8	32	668	112	248.6	91.9	19.707	-444.231	-485.303	-485.303
	27	3583.1	3609.8	32.2	666	111	247.5	91.9	19.715	-444.034	-485.12	-485.12
5*	1	19.4	32	21.7	661	111	249.7	92.7	12.943	-445.75	-486.709	-486.709
	2	99.1	117.5	21.7	659	110	250.3	92.7	12.896	-445.942	-486.887	-486.887
	3	198.6	203.8	22.4	658	110	249.5	92.4	12.969	-444.98	-485.996	-485.996
	4	298.2	303.7	21.7	657	111	249.7	91.3	12.873	-438.644	-480.314	-480.314
	5	852.7	863.2	23.4	2387	566	252.8	93.2	12.239	0	-73.9	-73.9
	6	1401.8	1408.2	16.3	163	38	251.8	92.8	0.673	-194.12	-253.675	-253.675
	7	1591.7	1599.7	19	724	154	253.1	92.7	3.086	-201.741	-260.732	-260.732
	8	1682.4	1687	14.6	75	17	254.6	93	0.341	-196.258	-255.654	-255.654
	9	1767.1	1773.8	17.8	372	84	255	92.6	1.568	-182.508	-242.921	-242.921
	10	1850.3	1855.7	13.4	58	15	254.5	92.5	0.265	-124.986	-189.649	-189.649
	11	1929.5	1936.2	17.8	208	48	254.2	92.4	0.937	-176.051	-236.941	-236.941
	12	2007.7	2013.5	17.6	56	14	255.1	92.6	0.336	-203.993	-262.818	-262.818
	13	2083.7	2089.6	16.3	164	40	257.8	92.7	0.77	-145.117	-208.293	-208.293
	14	2230	2235.9	15.5	66	17	257.9	92.8	0.372	-119.961	-184.996	-184.996
	15	3483.4	3493.6	31.8	630	105	249.5	92.5	18.574	-445.837	-486.79	-486.79
	16	3583.1	3603	32.2	630	105	247.1	92.4	18.659	-446.278	-487.198	-487.198

Peak number Start (s) RT (s) Width (s) Ampl. 2 (mV) Ampl. 3 (mV) BGD 2 (mV) BGD 3 (mV) Area all (Vs) rd T (permil) vs. C16 dT (permil) vs. C16 dD (permil) vs. VSMOW

Duplicate 1 (from Results 1)

Table with 11 columns: Peak number, Start (s), RT (s), Width (s), Ampl. 2 (mV), Ampl. 3 (mV), BGD 2 (mV), BGD 3 (mV), Area all (Vs), rd T (permil) vs. C16, dT (permil) vs. C16, dD (permil) vs. VSMOW. Rows 1-21.

Duplicate 2

Table with 11 columns: Peak number, Start (s), RT (s), Width (s), Ampl. 2 (mV), Ampl. 3 (mV), BGD 2 (mV), BGD 3 (mV), Area all (Vs), rd T (permil) vs. C16, dT (permil) vs. C16, dD (permil) vs. VSMOW. Rows 1-21.

Differences ...squared

Table with 2 columns: Differences, ...squared. Values for peaks 1-21.

Average = 254 5665881 RMS = 15 955143

Duplicate 3

Table with 11 columns: Peak number, Start (s), RT (s), Width (s), Ampl. 2 (mV), Ampl. 3 (mV), BGD 2 (mV), BGD 3 (mV), Area all (Vs), rd T (permil) vs. C16, dT (permil) vs. C16, dD (permil) vs. VSMOW. Rows 1-28.

Duplicate 4

Table with 11 columns: Peak number, Start (s), RT (s), Width (s), Ampl. 2 (mV), Ampl. 3 (mV), BGD 2 (mV), BGD 3 (mV), Area all (Vs), rd T (permil) vs. C16, dT (permil) vs. C16, dD (permil) vs. VSMOW. Rows 1-31.

C23
C25
C27
C29
AMPS
C23
C25
C27
C29
RETS
C16
C23
C25
C27
C29
C36

Triplicate 1

Table with 11 columns: Peak number, Start (s), RT (s), Width (s), Ampl. 2 (mV), Ampl. 3 (mV), BGD 2 (mV), BGD 3 (mV), Area all (Vs), rd T (permil) vs. C16, dT (permil) vs. C16, dD (permil) vs. VSMOW. Row 1.

H2a CONT

49	2672.7	2678.8	13	97	24	333.9	109.7	0.556	-163.839	-225.631	-225.631
50	2685.6	2692.8	13.8	149	36	333.9	109.7	1.11	-186.752	-246.851	-246.851
51	2699.4	2706.3	17.3	69	18	333.9	109.7	0.674	-201.291	-260.316	-260.316
52	2789.1	2794.7	16.7	60	16	330.8	108.8	0.299	-64.204	-133.36	-133.36
53	2806.5	2816	17.1	58	15	322.6	107.1	0.457	-170.91	-232.18	-232.18
54	2823.6	2833	16.5	65	16	322.6	107.1	0.648	-178.536	-239.242	-239.242
55	3483.8	3485.1	31.8	1006	169	256.4	94.3	29.705	-442.246	-483.464	-483.464
56	3583.3	3595.4	32.4	1004	169	253.9	93.7	29.78	-441.757	-483.012	-483.012
TriPLICATE 4											
1	16.5	20.5	25.5	1002	168	254.8	94.5	19.674	-445.75	-486.709	-486.709
2	99.1	100.3	22.8	997	168	257	94.1	19.548	-442.727	-483.91	-483.91
3	198.6	199.8	23.6	995	167	256	93.9	19.615	-442.271	-483.487	-483.487
4	298.2	299.3	21.7	993	167	254.5	94.1	19.455	-444.324	-485.388	-485.388
5*	877.8	882.8	42	4456	1113	259.4	95	34.296	0	-73.9	-73.9
6	997.3	1002.2	20.3	93	27	273.8	98.4	0.619	-22.906	-95.113	-95.113
7	1111.3	1116.7	10	130	36	274.8	98.1	0.504	-62.246	-131.546	-131.546
8	1222.2	1227.7	20.3	158	42	276.3	99.3	1.355	-149.261	-212.13	-212.13
9	1328.6	1335.1	19.6	150	37	280.8	100.6	1.375	-204.993	-263.744	-263.744
10	1428.3	1437.1	36.2	735	175	270.3	97.5	8.354	-212.071	-270.299	-270.299
11	1525.5	1533.4	32	389	95	272.9	97.7	5.439	-202.756	-261.672	-261.672
12	1617.5	1650.5	54.1	8855	2093	272.7	96.8	140.305	-227.886	-284.945	-284.945
13	1671.6	1675.1	31.6	147	32	272.7	96.8	3.228	-234.287	-290.873	-290.873
14	1703.1	1722	48.3	952	224	272.7	96.8	13.796	-216.323	-274.237	-274.237
15	1794.3	1831.7	58.9	10246	2477	292	101.4	186.757	-227.726	-284.797	-284.797
16	1853.2	1892.7	71.1	1243	292	292	101.4	19.347	-222.462	-279.922	-279.922
17	1958.3	2012	68.5	15243	3941	320.7	107.4	388.975	-225.461	-282.699	-282.699
18	2024.8	2033.8	17.6	176	40	320.7	107.4	1.823	-237.227	-293.596	-293.596
19	2043	2061.6	36.2	3611	737	361.6	116.6	28.36	-224.397	-281.714	-281.714
20	2116.1	2148.1	37	7509	1631	322	108.1	104.581	-219.354	-277.041	-277.041
21	2153.1	2154.8	17.8	438	92	322	108.1	3.672	-293.891	-345.887	-345.887
22	2170.9	2181.1	18.4	93	21	322	108.1	1.171	-283.523	-336.471	-336.471
23	2194.9	2207.9	23.4	2623	552	346.4	113	18.016	-219.505	-277.183	-277.183
24	2260.1	2278.9	28.6	2603	552	334.4	110.2	18.184	-205.383	-264.105	-264.105
25	2288.8	2293.6	13.4	184	43	334.4	110.2	1.188	-259.384	-314.116	-314.116
26	2305.5	2313.2	15.5	339	78	356.3	114.2	1.88	-212.098	-270.324	-270.324
27	2332.2	2341.4	18.4	497	119	338.2	111.2	2.504	-203.728	-262.573	-262.573
28	2353.3	2366.1	20.1	1191	243	353.2	114	7.205	-309.584	-309.584	-309.584
29	2380.7	2384.9	9.6	120	28	373.8	117.4	0.556	-188.607	-248.599	-248.599
30	2401.8	2409.4	18.8	836	193	353	114.4	4.134	-193.484	-253.086	-253.086
31	2420.6	2425.7	10.2	76	17	353	114.4	0.405	-285.176	-338.001	-338.001
32	2435.5	2439.4	10	70	17	358.2	115.3	0.357	-171.963	-233.062	-233.062
33	2460.6	2467.2	10.5	307	71	378.3	119.9	1.487	-214.135	-272.21	-272.21
34	2471	2472.1	9	106	22	378.3	119.9	0.315	-259.689	-314.398	-314.398
35	2518	2527	13.8	72	16	344.1	112.7	0.506	-231.026	-287.853	-287.853
36	2531.8	2536.8	13.8	220	55	344.1	112.7	1.118	-192.15	-251.85	-251.85
37	2547.9	2554	13	62	16	346.2	112	0.347	-103.661	-169.901	-169.901
38	2560.9	2568	15.5	86	22	346.2	112	0.642	-129.627	-193.948	-193.948
39	2576.3	2582.4	16.1	68	17	346.2	112	0.602	-114.983	-180.385	-180.385
40	2592.4	2599.8	15.9	145	37	346.2	112	0.975	-153.303	-215.874	-215.874
41	2656.6	2660.8	10.2	65	17	351.9	113.9	0.297	-150.093	-212.901	-212.901
42	2662.7	2690.7	13.6	55	14	344.3	112.2	0.386	-181.826	-242.29	-242.29
43	3094.8	3096.3	4	67	15	300.3	102.1	0.11	-181.49	-241.978	-241.978
44	3357.8	3372	30.7	53	16	279.4	97.4	0.814	-90.798	-157.988	-157.988
45	3483.6	3489	33.4	951	160	253.1	93.7	28.084	-444.107	-485.187	-485.187
46	3580.8	3584.4	34.9	947	159	252.8	93.7	28.106	-444.287	-485.355	-485.355
TriPLICATE 5											
1	19	20.5	22.2	929	156	256.2	94.3	18.2	-446.581	-487.479	-487.479
2	98.9	103.7	21.9	927	156	255.5	93.7	18.161	-444.181	-485.256	-485.256
3	198.6	216.7	23.2	924	155	255.4	94.5	18.238	-446.561	-487.46	-487.46
4	297.4	306.8	22.6	924	155	254.2	94.2	18.12	-446.998	-487.865	-487.865
5*	871.5	888.7	38	4222	1069	257.8	95.1	30.547	0	-73.9	-73.9
6	1218.9	1223.1	14.6	110	29	264.5	96.3	0.465	-112.42	-178.012	-178.012
7	1323.6	1328.4	16.9	124	31	264.7	96.6	0.513	-176.763	-237.6	-237.6
8	1422	1431	21.7	674	152	261.5	95.7	2.876	-195.712	-255.149	-255.149
9	1521.5	1527.2	25.5	335	62	262.4	95.4	1.943	-184.631	-244.886	-244.886
10	1611.9	1634.6	36.4	5136	1074	263.3	95.3	50.736	-223.742	-281.106	-281.106
11	1648.2	1653.6	15.3	85	18	263.3	95.3	0.884	-274.055	-327.702	-327.702
12	1704	1711.5	28.2	476	115	278.2	98.9	4.319	-216.248	-274.167	-274.167
13	1787.8	1814.1	53.5	5978	1295	270.5	97.1	69.34	-226.583	-283.739	-283.739
14	1874.1	1882.5	24.2	695	165	281.3	99.1	6.07	-210.831	-269.151	-269.151
15	1952.5	1988	58.9	8955	2052	278.5	98.6	146.333	-226.403	-283.572	-283.572
16	2033.4	2046.1	25.1	1795	378	298.6	102	10.36	-215.18	-273.178	-273.178
17	2108.2	2129.5	30.1	4040	854	283.4	99.1	38.548	-216.655	-274.544	-274.544
18	2138.3	2144.5	13.6	127	27	283.4	99.1	1.135	-297.639	-349.543	-349.543
19	2184.1	2194.7	22.2	1278	269	291.4	100.7	6.521	-212.407	-270.61	-270.61
20	2257	2266.6	20.9	1245	266	289.4	100.5	6.133	-199.775	-258.911	-258.911
21	2277.9	2282.9	13.8	61	13	289.4	100.5	0.372	-305.125	-356.476	-356.476
22	2293.3	2301.1	16.9	129	30	284.8	101.2	0.631	-206.99	-285.594	-285.594
23	2327	2332.6	13.4	184	47	286.7	97.8	0.847	-67.63	-155.054	-155.054
24	2345.8	2353.1	17.3	536	118	295.3	101.4	2.465	-238.855	-295.103	-295.103
25	2394.1	2401.2	19.9	308	75	288.9	98.8	1.455	-170.488	-231.789	-231.789
26	2453	2457.8	10	120	29	303.1	103.5	0.47	-193.679	-253.267	-253.267
27	2526.6	2531.4	12.7	67	18	297.8	101.7	0.296	-84.208	-151.885	-151.885
28	3483	3488.6	32.6	890	148	251.1	93.9	26.254	-448.436	-489.197	-489.197
29	3582.9	3589.8	32.2	884	148	252.2	94.4	26.208	-449.279	-489.978	-489.978

	T1	T2	T3	T4	T5	Average	std dev
C23		-263.4	-272.962			-268.181	6.761355042
C25	-252.746	-282.3	-284.238	-284.495	-281.108	-283.03525	1.615793175
C27	-257.347	-279.842	-279.197	-284.797	-283.739	-278.9844	2.787827514
C29	-256.768	-277.839	-274.52	-282.699	-283.572	-275.0796	4.253425326

AMPS	T1	T2	T3	T4	T5
C23		1172	1175		
C25	1479	6955	14735	8855	5136
C27	1391	6402	15647	10246	5978
C29	1834	8003	22154	15243	5978

	T1	T2	T3	T4	T5	Average	std dev
C23		-272.217	-281.737			-276.9786653	6.731533076
C25	-257.725	-261.739	-251.292	-259.9497382	-265.5489446	-259.2508084	6.030858044
C27	-263.338	-260.648	-245.26	-257.8446977	-265.6754648	-258.5531212	8.691102397
C29	-258.197	-254.963	-234.846	-249.1934258	-265.5084648	-252.5416339	12.78468843

RETs	T1	T2	T3	T4	T5
C16	879.1	896.8	900.8		892.8
C23		1584.8	1444.6		
C25	1892.7	1943.7	1670.7	1650.5	1634.8
C27	2199.1	2252.4	1854	1831.7	1814.1
C29	2495.5	2562.3	2040.7	2012	1988
C36	4033	4033	2827	2827	2827

Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs. VSMOW
Duplicate 1											
1	19.4	20.5	22.2	2134	359	33.1	25.7	40.696	-434.01	-475.836	-475.836
2	99.1	100.1	22.2	2113	356	33.1	25.6	40.371	-433.993	-475.821	-475.821
3	198.6	199.6	22.4	2106	352	33.2	26	40.219	-434.661	-476.439	-476.439
4	298	299.1	22.2	2098	349	33.2	25.3	39.556	-433.504	-475.368	-475.368
5	510.8	530.7	99.1	2609	739	41.6	27.8	55.473	-27.113	-99.009	-99.009
6*	1142	1172.1	78.8	1645	471	86.3	40.1	42.798	0	-73.9	-73.9
7	1275.1	1325.9	84.2	175	47	112.7	48	8.301	-111.367	-177.037	-177.037
8	1420.4	1459.9	77.3	169	42	153.8	58.4	5.422	-153.925	-216.45	-216.45
9	1587.4	1625	105.5	362	85	150.5	57.5	17.256	-168.986	-230.398	-230.398
10	1694.6	1791.3	129.2	372	90	183.2	64.4	17.781	-277.853	-331.034	-331.034
11	1823.7	1870.3	98.4	1456	291	183.2	64.4	52.577	-299.805	-351.549	-351.549
12	1922.2	1954.4	103.9	660	151	183.2	64.4	20.95	-186.081	-246.229	-246.229
13	2036.1	2117	177.9	441	103	137.3	53.3	21.815	-192.388	-252.071	-252.071
14	2239.9	2288.1	122.1	1197	271	108	45.7	47.901	-211.143	-269.439	-269.439
15	2398.3	2444.9	113.7	919	209	127.9	49.5	37.327	-209.944	-268.329	-268.329
16	2550.4	2615.2	137.9	2247	509	101.6	43	99.05	-217.315	-275.155	-275.155
17	2703.8	2756.3	143.4	1179	270	137.2	51.3	55.729	-214.543	-272.588	-272.588
18	2847.8	2928.3	148.8	3366	779	152.3	53.1	171.217	-213.058	-271.213	-271.213
19	2996.6	3058.5	131.3	2014	465	152.3	53.1	97.304	-207.06	-265.659	-265.659
20	3128.5	3227	134.8	4493	1069	150.4	54.6	260.056	-211.404	-269.681	-269.681
21	3263.3	3330.2	131.5	2160	490	150.4	54.6	110.361	-212.681	-270.864	-270.864
22	3394.8	3486.6	135.1	4361	1050	150.4	54.6	254.744	-203.199	-262.063	-262.063
23	3530.8	3588.5	78.8	1732	392	150.4	54.6	84.552	-212.824	-271.089	-271.089
24	3609.6	3634.9	42.2	1457	319	150.4	54.6	43.194	-241.017	-297.108	-297.108
25	3651.9	3720	114.1	3703	889	150.4	54.6	191.529	-191.397	-251.153	-251.153
26	3786	3804.4	104.5	1221	276	150.4	54.6	47.867	-210.945	-269.256	-269.256
27	3871.1	3906	107	1091	250	197.7	65.3	37.897	-192.556	-252.226	-252.226
28*	3978.1	4022	105.8	1657	382	197.7	65.3	50.505	0	-244.1	-244.1
29	4084.5	4155.8	111.6	128	30	149	54.8	8.014	-16.843	-256.832	-256.832
30	4996.6	4997.4	101.6	1315	209	53.6	31.7	122.019	-313.286	-480.913	-480.913
31	5115.9	5116.9	62.1	1285	209	33.5	25.6	73.639	-305.488	-475.018	-475.018
Duplicate 2											
1	19.4	20.3	21.9	1246	201	33.3	25.5	23.411	-437.519	-479.086	-479.086
2	99.1	99.9	21.7	1239	198	33.3	25.5	23.223	-437.747	-479.297	-479.297
3	198.6	199.4	21.9	1215	197	33.3	25.6	23.125	-437.963	-479.498	-479.498
4	298	299.1	21.9	1195	195	33.3	25.5	22.772	-437.606	-479.167	-479.167
5	510.8	530.9	99.9	2587	733	43	28.2	54.951	-21.633	-93.935	-93.935
6*	1143	1171.9	77.5	1639	469	87.9	41.1	43.305	0	-73.9	-73.9
7	1275.3	1324.2	86.1	185	49	117.4	49.2	8.875	-104.458	-170.639	-170.639
8	1419.7	1460.1	79.6	172	41	160.9	61.2	5.724	-187.527	-247.569	-247.569
9	1588.6	1626.9	104.5	369	87	150.4	59.4	18.315	-166.062	-227.69	-227.69
10	1694.6	1791.3	130.4	380	82	192.4	67.4	18.983	-289.428	-341.939	-341.939
11	1825	1871.4	97.8	1505	302	192.4	67.4	56.409	-300.635	-352.318	-352.318
12	1922.8	1954.2	104.9	672	154	192.4	67.4	22.814	-192.99	-252.628	-252.628
13	2036.5	2116.8	180.2	449	104	144.7	55.6	23.338	-201.741	-260.732	-260.732
14	2240.7	2287.9	122.1	2287	92	112.4	46.7	51.526	-207.904	-266.44	-266.44
15	2399.1	2444.5	114.3	942	215	133.8	51.3	40.29	-210.577	-268.915	-268.915
16	2551.9	2616.5	152.6	2349	535	105.6	43.6	107.157	-211.957	-270.193	-270.193
17	2705.7	2756.3	143.4	1240	284	144.7	53.5	60.53	-216.058	-273.992	-273.992
18	2849.5	2930.6	149.6	3558	826	160.3	55.1	183.077	-210.489	-268.834	-268.834
19	2999.6	3059.1	131.5	2034	469	235.3	75.1	93.681	-215.709	-273.668	-273.668
20	3131.9	3229.3	133.6	4591	1098	159.7	56.5	268.699	-208.475	-266.968	-266.968
21	3265.4	3330.6	132.5	2168	493	159.7	56.5	113.226	-208.298	-266.805	-266.805
22	3397.9	3487.8	132.3	4188	1006	159.7	56.5	242.309	-200.868	-259.924	-259.924
23	3530.2	3587.7	123.3	1594	360	159.7	56.5	130.659	-222.018	-279.511	-279.511
24	3653.5	3714.6	110.8	3319	793	159.7	56.5	165.903	-190.134	-249.983	-249.983
25	3764.3	3817.4	107.2	1188	267	159.7	56.5	48.549	-210.027	-268.406	-268.406
26	3872.1	3901.8	84	943	214	212.7	68.9	27.033	-194.233	-253.779	-253.779
27*	3978.9	4023	104.9	1368	399	238.3	75	51.6	0	-244.1	-244.1
28	4085.3	4102	28.8	71	17	161.4	58.1	1.212	-7.856	-250.038	-250.038
29	4114.8	4152.6	79.4	111	26	194.5	65.7	4.097	-19.739	-259.021	-259.021
30	4996.4	4997.4	101.6	765	119	58	33	70.611	-333.564	-496.241	-496.241
31	5115.9	5116.7	61.9	751	120	33.5	25.4	43.304	-314.77	-482.034	-482.034
peak	start	ret	width	amp2	amp3	back 2	back 3	area all	rd 3h2/2h2	d 2h/1h	
1	19.4	31.4	21.9	614	103	250.8	92.5	12.02	-440.485	-481.833	
2	98.4	109.9	22.4	613	102	249.7	92.8	11.994	-444.518	-485.568	
3	198.6	207.1	21.7	611	102	249.8	92.7	12.045	-443.841	-484.941	
4	298	300.3	21.9	611	101	248.6	92.6	11.961	-444.208	-485.281	
5*	849.2	862.8	30.9	2489	610	265	96.8	14.042	0	-73.9	
6	902.9	914	18.1	84	23	281	101.1	0.529	-87.921	-153.323	
7	919	922.3	10.2	69	19	281	101.1	0.377	-48.732	-119.031	
8	966.6	976.9	23.8	247	64	303.2	106.8	2.321	-110.064	-175.83	
9	990.5	996.1	22.2	456	125	303.2	106.8	2.898	-46.123	-116.615	
10	1076.8	1092.9	36.4	262	69	356.4	122	4.499	-145.038	-208.22	
11	1113.1	1114.4	11.3	78	18	356.4	122	0.665	-232.806	-289.501	
12	1124.4	1128.4	10	56	14	356.4	122	0.421	-181.447	-241.939	
13	1197.2	1204.7	18.4	687	163	405.4	133.7	6.219	-175.487	-236.418	
14	1216	1221.8	29.9	215	62	691.3	200.7	-0.869	-670.082	-694.463	
15	1265.3	1270.7	11.1	59	13	482.2	149.6	0.307	-266.703	-320.894	
16	1278.4	1282.6	12.7	129	30	482.2	149.6	0.895	-209.435	-267.858	
17	1289.1	1295.8	15.7	388	81	482.2	149.6	3.231	-277.012	-330.441	
18	1304.8	1311.3	23.8	491	114	482.2	149.6	7.3	-217.146	-274.999	
19	1328.6	1343.7	20.3	2736	527	482.2	149.6	27.366	-286.519	-339.246	
20	1348.9	1349.5	30.3	1265	281	482.2	149.6	15.885	-318.357	-368.73	
21	1379.2	1384.2	24.7	85	22	482.2	149.6	0.551	75.758	-3.741	
22	1403.9	1412.6	57.9	878	210	482.2	149.6	18.899	-166.931	-228.495	
23	1473	1486	27.2	137	36	404.9	133.2	2.639	-103.324	-169.588	
24	1500.2	1514.4	31.8	672	161	404.9	133.2	13.887	-187.427	-247.476	
25	1592.8	1607.6	66.3	1788	423	368.6	123.5	44.24	-215.059	-273.066	C23
26	1682.7	1696.9	58.1	1446	340	389.3	127.3	34.6	-214.035	-272.118	
27	1767.3	1788.6	66.9	3454	824	348.6	117	89.924	-224.062	-281.422	C25
28	1834.2	1869.5	68	1871	442	348.6	117	57.009	-221.932	-279.432	
29	1932.5	1962.5	67.1	5456	1324	348.6	117	156.157	-228.911	-285.864	C27
30	1999.3	2035.7	66.1	3146	749	348.6	117	95.028	-226.146	-283.333	
31	2085.4	2132	64.8	9919	2522	348.6	117	254.342	-227.424	-284.517	C29
32	2150.2	2152.9	19.4	1406	315	348.6	117	15.806	-238.927	-295.17	
33	2189.6	2190.5	49.5	3369	802	348.6	117	82.846	-226.108	-283.299	
34	2223.8	2284.6	64	10507	2565	561.9	164	230.985	-213.476	-271.6	
35	2287.7	2289.6	7.9	2260	527	561.9	164	11.925	-212.551	-270.743	
36	2295.9	2309.4	24.5	476	107	1374	349.4	4.434	-280.499	-333.67	
37	2320.3	2341.4	25.7	5009	1133	1374	349.4	40.419	-184.893	-245.129	
38	2346	2362.1	20.3	1978	402	1					

CO2 CONT

47	2558.6	2563.2	13.4	128	32	664.3	186.3	-0.387	-426.17	-468.576	
48	2572	2578.9	16.1	181	47	664.3	186.3	-1.029	-349.031	-397.138	
49	2588.7	2594.7	13	67	18	449.2	137.7	0.295	-15.905	-88.63	
50	2625.5	2639.3	21.9	551	131	407.1	128.7	3.723	-174.37	-235.384	
51	2647.4	2655.1	13.6	373	89	407.1	128.7	2.763	-183.164	-243.528	
52	2661	2667.9	14	481	115	407.1	128.7	4.239	-192.991	-252.629	
53	2675	2680.4	14	228	54	407.1	128.7	2.168	-214.71	-272.743	
54	2691.1	2696.9	14.8	94	25	455.5	138.9	0.183	199.088	110.475	
55	2755.2	2762.4	17.1	151	37	379.2	122	0.956	-141.588	-205.025	
56	2772.4	2781.6	16.3	180	44	379.2	122	1.382	-169.262	-230.654	
57	2788.7	2798.3	17.1	226	55	379.2	122	2.277	-189.558	-249.449	
58	2805.8	2812.5	18.8	75	17	379.2	122	0.919	-235.716	-292.196	
59	2913.5	2924.5	23	123	30	331.8	111.2	1.046	-201.577	-260.58	
60	2936.9	2950.7	23.2	200	48	321.5	108.1	2.157	-170.768	-232.048	
61	2960.1	2971.4	21.9	191	46	321.5	108.1	2.522	-187.788	-247.811	
62	2982	2993.7	25.1	60	14	321.5	108.1	1.089	-221.722	-279.237	
63	3135	3149.2	30.1	137	16	295.5	101.5	0.722	-117.977	-163.158	
64	3108.0	3185.6	30.3	62	34	292.3	100.9	2.159	-159.634	-221.737	
65	3199	3219	32.8	202	47	292.3	100.9	3.804	-195.982	-255.399	
66	3481.3	3487.6	34.5	586	96	246.7	91.7	17.366	-437.525	-479.092	
67	3583.1	3611.1	33.2	586	96	247.7	92.8	17.37	-442.593	-483.786	
5*	1	15.9	35.7	25.5	581	248.7	92.6	11.39	-445.465	-486.445	
	2	97.8	104.9	23	579	248.9	92.4	11.351	-443.111	-484.265	
	3	197.9	204.4	22.8	577	250.6	93.1	11.379	-446.872	-487.748	
	4	298.2	313.9	22.4	576	251	93.4	11.293	-446.834	-487.713	
	6	847.9	860.5	28	2635	252.6	93.3	14.446	0	-73.9	
	7	1193.6	1198.2	18	139	259.8	95.7	0.572	-184.851	-245.09	
	8	1284.3	1288.7	14	73	265.4	96.7	0.289	-260.724	-315.357	
	9	1298.3	1303.5	13.2	83	265.4	96.7	0.347	-180.693	-241.239	
	8	1323	1330.1	16.9	616	263.5	96	2.519	-267.539	-321.988	
	10	1397.8	1404.9	17.1	359	259.9	95.3	1.248	-178.973	-237.798	
	11	1496	1501.5	17.1	219	261.3	95.3	0.909	-157.52	-219.78	
	12	1586.9	1595.7	18.6	606	258.6	94.4	2.541	-180.964	-241.491	
	13	1677.4	1684.7	19.6	525	256.6	94.3	2.234	-200.685	-259.754	
	14	1760.8	1773.2	26.1	1184	242	255.8	93.7	5.785	-212.16	-270.381 C25
	15	1846.9	1854.7	21.9	765	260	94.2	3.394	-197.366	-256.681	
	16	1925.5	1938.9	23.4	1873	261.5	94.7	10.956	-217.945	-275.739 C27	
	17	2003.3	2015.2	23	1298	268	95.4	6.792	-216.055	-273.988	
	18	2081.6	2096.1	23.4	2603	268	96.2	18.438	-217.854	-275.654 C29	
	19	2105	2111.3	17.1	505	268	96.2	2.673	-260.932	-315.549	
	20	2154	2165.7	21.9	1258	271	96.6	6.465	-216.813	-274.69	
	21	2212.1	2217.3	15.5	80	284.7	100.2	0.293	-302.706	-354.236	
	22	2227.5	2243.8	25.3	2659	284.7	100.2	20.332	-212.065	-270.293	
	23	2252.8	2256.2	9.4	95	284.7	100.2	0.522	-319.714	-369.987	
	24	2252.2	2269.9	20.5	374	284.7	100.2	2.072	-262.579	-317.075	
	25	2298	2307.6	16.9	1005	285.5	99.4	5.131	-206.251	-264.909	
	26	2314.9	2322	18.6	581	285.5	99.4	2.988	-262.277	-316.795	
	27	2333.5	2345	20.9	154	285.5	99.4	1.098	-236.968	-293.356	
	28	2364.8	2381.1	24.2	2423	280.9	96.7	16.68	-197.804	-257.086	
	29	2389.1	2392.6	9.6	89	280.9	96.7	0.583	-250.689	-306.063	
	30	2422.7	2429.2	11.9	340	332.1	111.2	1.645	-243.711	-299.801	
	31	2434.6	2440.3	17.3	334	332.1	111.2	1.654	-279.868	-333.086	
	32	2497.8	2506.1	18	650	302.7	103.2	3.161	-192.784	-252.437	
	33	2515.7	2521.4	13.6	51	302.7	103.2	0.315	-230.6	-287.459	
	34	2620.9	2628.4	16.1	70	295.9	102.1	0.375	-188.968	-248.903	
	35	2971.6	3013.4	65.2	99	303	103.6	3.548	-197.648	-256.942	
	36	3481.9	3488.8	34.7	555	246.7	92.5	16.389	-445.124	-486.129	
	37	3583.1	3595.4	32.4	552	247.5	92.9	16.337	-447.263	-488.128	
5*	1	19.4	29.9	22.2	976	251.4	93.6	19.148	-440.537	-481.882	
	2	99.1	109.5	21.7	974	250.7	93.5	19.086	-440.281	-481.644	
	3	198.6	217.4	22.2	970	248	93	19.126	-440.416	-481.769	
	4	297.4	310.2	22.6	967	247	93.2	18.972	-442.936	-484.103	
	6	850.6	861.5	30.7	2595	253.7	93.9	14.07	0	-73.9	
	7	1195.1	1199.5	15.5	103	258.9	95.1	0.429	-131.485	-195.669	
	8	1285.8	1289.9	10.9	57	262	96.1	0.228	-227.759	-284.828	
	9	1300.6	1304.8	14.6	62	262.8	95.9	0.274	-114.36	-179.809	
	10	1323.8	1330.9	15.9	477	261.6	95.7	1.935	-262.734	-317.218	
	11	1399.9	1405.7	17.8	55	257.8	95.1	0.951	-197.465	-256.772	
	12	1495.4	1502.5	17.1	161	260.6	93.9	0.866	-35.692	-106.955	
	13	1588.2	1596.3	19.9	468	258.4	94.3	1.912	-172.905	-234.027	
	14	1678.3	1685.4	17.8	307	254.3	93.8	1.65	-190.4	-250.23	
	15	1764.4	1773.4	19	935	253.7	93	4.195	-198.961	-258.158	
	16	1765.8	1773.4	15.3	935	253.7	93	4.148	-198.37	-258.537	
	17	1846.3	1855.1	21.5	592	255.7	93.6	2.518	-194.48	-254.008	
	18	1927.2	1938.7	22.8	1531	255.9	93.7	8.125	-217.65	-275.466 C27	
	19	2005.8	2015	21.7	1031	261.7	94.7	4.961	-211.739	-269.991	
	20	2076.4	2095.4	29.1	2200	262.1	94.5	13.759	-213.511	-271.633 C29	
	21	2105.5	2111.7	18	385	262.1	94.5	2.02	-252.769	-307.989	
	22	2156	2165.9	20.3	962	265.8	95.3	4.823	-211.441	-269.716	
	23	2212.7	2218.1	13.6	60	276.1	97.6	0.248	-207.604	-266.162	
	24	2229.2	2243.2	24	2273	271.1	96.1	15.247	-207.473	-266.041	
	25	2253.2	2256.8	9.2	69	271.1	96.1	0.4	-286.07	-338.83	
	26	2262.4	2270.2	21.1	275	271.1	96.1	1.543	-237.752	-294.083	
	27	2297.5	2307.8	18.2	793	271.6	96.4	3.794	-203.991	-262.816	
	28	2315.7	2322.2	17.3	433	271.6	96.4	2.184	-260.976	-315.59	
	29	2336.2	2345.6	19	106	277.4	97.4	0.776	-199.185	-258.366	
	30	2366.5	2380.7	22.8	1960	273.9	96.3	12.412	-191.782	-251.509	
	31	2389.3	2393.1	10.7	57	273.9	96.3	0.369	-255.496	-310.514	
	32	2417.7	2429.2	17.6	241	283.7	99.2	1.195	-234.481	-291.053	
	33	2435.3	2440.5	17.1	235	283.7	99.2	1.004	-212.67	-270.854	
	34	2498.4	2505.9	18.6	497	277.2	97.6	2.327	-178.138	-238.874	
	35	2620.9	2629	13.8	59	280.6	98.7	0.337	-146.478	-209.553	
	36	3482.4	3509.5	33.9	923	245.8	92.7	27.285	-441.835	-483.083	
	37	3583.1	3613.2	32.2	920	246.3	93	27.266	-443.024	-484.165	
5*	1	19.4	30.9	22.2	907	252.7	93.8	17.761	-441.32	-482.606	
	2	99.1	112.9	21.9	904	250.3	93.5	17.714	-441.522	-482.793	
	3	198.3	210.3	22.4	903	246.9	92.9	17.829	-442.449	-483.652	
	4	298.2	311.6	21.9	901	247.1	92.9	17.659	-441.685	-482.944	
	6	849	861.7	29.1	2528	253.8	93.9	13.462	0	-73.9	
	7	1195.5	1200.1	15.5	125	262	96.3	0.512	-166.446	-228.046	
	8	1286	1290.6	12.1	68	262.5	96	0.262	-171.574	-232.794	
	9	1300.2	1305.2	16.3	76	263	96.1	0.314	-125	-189.662	
	10	1324.9	1331.5	17.1	572	261.5	95.8	2.254	-268.7	-322.743	
	11	1400.3	1406.6	18.2	277	257.5	94.5	1.102	-153.789	-216.524	
	12	1495.8	1503.1	20.3	191	256.2	94.6	0.811	-167.142	-228.69	
	13	1590.5	1597.2	17.3	542	258.4	94.9	2.224	-195.285	-254.754	
	14	1678.5	1686.4	20.7	467	258.7	94.4	1.943	-182.477	-242.892	
	15	1765.9	1774.4	24.2	1106	229	256.4	93.6	5.079	-206.527	-265.165
	16	1765.8	1774.4	19.6	1106	229	256.4	93.6	5.017	-204.864	-263.624 C25
	17	1848.4	1856.1	20.5	682	260.1	94.6	2.993	-200.37	-259.463	
	18	1927.8	1939.9	23.6	1758	260.8	94.4	9.577	-215.724	-273.882 C27	
	19	2006.4	2016.2	20.5	1190	263.1	95	5.921	-213.806	-271.906	
	20	2076.6	2096.7	29.5	2403	264.6	95.1	16.191	-214.866	-272.887 C29	
	21	2106.1	2112.4	17.1	447	264.6	95.1	2.351	-251.628	-306.933	

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peak	start	ret	width	amp2	amp3	back 2	back 3	area all	rd 3h2/2h2	d 2h/1h		
20	2155.8	2186.5	21.3	1124	237	289	96.3	5.888	-216.1	-274.03		
21	2213.5	2218.3	15.7	71	16	281.3	96.7	0.247	-214.833	-272.857		
22	2229.2	2244.2	24.5	2570	515	281.3	96.7	17.843	-210.573	-268.912		
23	2253.6	2257	9.2	76	16	281.3	96.7	0.396	-279.53	-332.773		
24	2282.8	2270.8	20.5	320	70	281.3	96.7	1.864	-254.11	-309.231		
25	2299.6	2308.4	16.5	918	199	271.4	97	4.508	-213.604	-271.719		
26	2316.1	2322.8	19.9	516	108	271.4	97	2.894	-275.03	-328.805		
27	2336	2346	19.4	142	31	271.4	97	1.108	-278.228	-331.567		
28	2367.8	2381.6	21.9	2245	455	276.5	97.2	14.843	-197.418	-258.729		
29	2389.7	2383.5	10.2	89	15	276.5	97.2	0.413	-285.705	-336.491		
30	2418.1	2429.8	17.3	309	68	288.7	100	1.499	-222.598	-280.048		
31	2435.5	2440.9	15.3	277	64	288.7	100	1.24	-208.096	-264.737		
32	2498.6	2506.3	18.2	572	132	283.1	98.8	2.751	-196.119	-246.285		
33	2621.7	2628.6	13.2	68	17	296.1	102	0.377	-123.876	-188.621		
34	3483.4	3492	33.4	864	145	250.3	93.4	25.533	-442.398	-483.605		
35	3583.1	3608.6	31.8	862	146	249	93.2	25.576	-442.185	-483.389		
5*	1	19.4	31.4	21.9	614	103	250.8	92.5	12.02	-440.485	-481.833	-481.833
	2	98.4	109.9	22.4	613	102	249.7	92.8	11.994	-444.518	-485.588	-485.588
	3	188.6	207.1	21.7	125	102	249.8	92.7	12.045	-443.841	-484.941	-484.941
	4	296	300.3	21.9	611	101	248.6	92.6	11.981	-444.208	-485.281	-485.281
	6	849.2	862.8	30.9	2489	610	285	98.8	14.042	0	-73.9	-73.9
	7	919	922.3	10.2	84	23	281	101.1	0.529	-87.921	-155.323	-155.323
	8	966.6	976.9	23.8	69	19	281	101.1	0.377	-48.732	-119.031	-119.031
	9	990.5	996.1	22.2	247	64	303.2	106.8	2.321	-110.064	-175.83	-175.83
	10	1076.8	1092.9	36.4	456	125	303.2	106.8	2.898	-46.123	-116.615	-116.615
	11	1113.1	1114.4	11.3	262	69	356.4	122	4.499	-145.038	-208.22	-208.22
	12	1124.4	1128.4	10	78	18	356.4	122	0.865	-232.806	-289.501	-289.501
	13	1197.2	1204.7	18.4	56	14	356.4	122	0.421	-181.447	-241.939	-241.939
	14	1216	1221.8	29.9	687	163	405.4	133.7	8.219	-175.487	-236.418	-236.418
	15	1253.3	1270.7	11.1	216	62	691.3	200.7	-0.869	-870.082	-694.463	-694.463
	16	1278.6	1282.6	12.7	59	13	482.2	149.6	0.307	-268.703	-320.894	-320.894
	17	1289.1	1296.8	15.7	442	90	482.2	149.6	0.895	-209.435	-267.858	-267.858
	18	1304.8	1311.3	23.8	388	81	482.2	149.6	3.231	-277.012	-330.441	-330.441
	19	1328.6	1343.7	20.3	491	114	482.2	149.6	7.3	-274.999	-274.999	-274.999
	20	1348.9	1349.5	30.3	2738	527	482.2	149.6	27.366	-286.519	-339.246	-339.246
	21	1379.2	1384.2	24.7	1265	261	482.2	149.6	15.885	-318.357	-368.73	-368.73
	22	1403.9	1412.6	57.9	85	22	482.2	149.6	0.551	75.758	-3.741	-3.741
	23	1473	1486	27.2	878	210	482.2	149.6	18.899	-166.931	-228.495	-228.495
	24	1500.2	1514.4	31.8	137	36	404.9	133.2	2.639	-103.324	-169.588	-169.588
	25	1592.8	1607.6	66.3	872	161	404.9	133.2	13.887	-187.427	-247.476	-247.476
	26	1682.7	1696.9	58.1	1788	423	368.6	123.5	44.24	-215.059	-273.086	-273.086
	27	1767.3	1786.6	66.9	1446	340	389.3	127.3	34.6	-214.035	-272.118	-272.118
	28	1834.2	1869.5	66.9	3454	924	348.6	117	89.924	-224.882	-281.422	-281.422
	29	1932.2	1952.5	87.1	1971	442	348.6	117	57.099	-221.932	-278.432	-278.432
	30	1969.3	2035.7	86.1	5450	1324	348.6	117	156.157	-228.911	-285.894	-285.894
	31	2085.4	2132	64.8	3148	740	348.6	117	95.028	-228.146	-283.333	-283.333
	32	2150.2	2152.9	19.4	9919	2522	348.6	117	254.342	-227.424	-284.517	-284.517
	33	2169.6	2190.5	49.5	1408	315	348.6	117	15.808	-238.927	-295.17	-295.17
	34	2223.8	2284.6	64	3369	802	348.6	117	82.846	-228.108	-283.299	-283.299
	35	2287.7	2289.6	7.9	10507	2565	561.9	164	230.985	-213.476	-271.6	-271.6
	36	2296.9	2309.4	24.5	2260	527	561.9	164	11.925	-212.551	-270.743	-270.743
	37	2320.3	2341.4	25.7	478	107	1374	349.4	4.434	-280.499	-333.87	-333.87
	38	2346	2362.1	20.3	5009	1133	1374	349.4	40.419	-184.893	-245.129	-245.129
	39	2366.3	2377.8	15.9	1978	402	1374	349.4	23.34	-251.875	-307.161	-307.161
	40	2382.2	2418.5	39.1	559	111	1374	349.4	-0.032	875.383	551.581	551.581
	41	2421.3	2422.9	7.7	8211	2027	1374	349.4	139.811	-171.758	-232.965	-232.965
	42	2440.9	2425.8	38.7	197	44	1374	349.4	0.827	98.925	17.714	17.714
	43	2489.4	2453.8	12.7	4988	927	855.3	185.9	141.568	-224.078	-281.419	-281.419
	44	2502.1	2527.4	30.1	60	16	545	160.4	0.212	-59.572	-129.07	-129.07
	45	2532.2	2537.5	11.5	3609	796	545	160.4	34.648	-198.444	-257.679	-257.679
	46	2543.7	2550.6	13.6	799	184	545	160.4	4.3	-202.883	-261.79	-261.79
	47	2558.6	2563.2	13.4	800	137	545	160.4	4.226	-207.83	-266.186	-266.186
	48	2572	2578.9	16.1	128	32	664.3	186.3	-0.387	-426.17	-468.576	-468.576
	49	2588.7	2594.7	13	181	47	664.3	186.3	-1.029	-349.031	-397.138	-397.138
	50	2625.5	2639.3	21.9	87	18	449.2	137.7	0.295	-15.905	-88.63	-88.63
	51	2647.4	2655.1	13.6	551	131	407.1	128.7	3.723	-174.37	-235.384	-235.384
	52	2661	2667.9	14	373	89	407.1	128.7	2.763	-183.164	-243.528	-243.528
	53	2675	2680.4	14	481	115	407.1	128.7	4.239	-162.991	-252.629	-252.629
	54	2691.1	2696.9	14.8	228	54	407.1	128.7	2.168	-272.743	-272.743	-272.743
	55	2755.2	2762.4	17.1	94	25	455.5	139.9	0.183	199.088	110.475	110.475
	56	2772.4	2781.6	16.3	151	37	379.2	122	0.958	-141.588	-205.025	-205.025
	57	2788.7	2798.3	17.1	180	44	379.2	122	1.382	-169.282	-230.654	-230.654
	58	2805.8	2812.5	16.8	228	55	379.2	122	2.277	-189.558	-249.449	-249.449
	59	2913.5	2924.5	23	75	17	379.2	122	0.919	-235.716	-292.196	-292.196
	60	2936.9	2950.7	23.2	123	30	331.8	111.2	1.046	-201.577	-260.58	-260.58
	61	2960.1	2971.4	21.9	200	48	321.5	108.1	2.157	-170.768	-232.048	-232.048
	62	2982	2993.7	25.1	191	46	321.5	108.1	2.522	-187.788	-247.811	-247.811
	63	3136	3149.2	30.1	60	14	321.5	108.1	1.089	-221.722	-279.237	-279.237
	64	3168.6	3185.6	30.3	82	16	295.5	101.5	0.722	-117.977	-183.158	-183.158
	65	3199	3219	32.8	137	34	292.3	100.9	2.159	-159.634	-221.737	-221.737
	66	3481.3	3487.6	34.5	202	47	292.3	100.9	6.604	-195.982	-255.399	-255.399
	67	3583.1	3611.1	33.2	588	99	248.7	91.7	17.366	-437.525	-479.092	-479.092
					98	98	247.7	92.8	17.37	-442.593	-483.786	-483.786
5*	1	15.9	35.7	25.5	581	98	248.7	92.6	11.39	-445.465	-486.445	-486.445
	2	97.8	104.9	23	579	97	248.7	92.4	11.351	-443.111	-484.265	-484.265
	3	197.9	204.4	22.8	577	96	250.6	93.1	11.379	-446.872	-487.748	-487.748
	4	298.2	313.9	22.4	576	96	251	93.4	11.293	-448.834	-487.713	-487.713
	6	847.9	860.5	28	2835	636	252.6	93.3	14.446	0	-73.9	-73.9
	7	1193.6	1198.2	18	139	34	258.8	95.7	0.572	-184.851	-245.09	-245.09
	8	1284.3	1288.7	14	73	17	265.4	96.7	0.289	-269.724	-315.357	-315.357
	9	1298.3	1303.5	13.2	83	21	265.4	96.7	0.347	-180.693	-241.239	-241.239
	10	1323	1330.1	16.9	618	119	263.5	96	2.519	-287.539	-321.668	-321.668
	11	1367.8	1404.9	17.1	309	73	259.9	95.3	1.248	-178.977	-237.798	-237.798
	12	1496	1501.5	17.1	219	53	261.3	95.3	0.909	-157.52	-219.78	-219.78
	13	1586.9	1595.7	16.6	608	134	258.6	94.4	2.541	-180.984	-241.491	-241.491
	14	1677.4	1684.7	19.6	525	116	256.6	94.3	2.234	-200.685	-259.754	-259.754
	15	1760.8	1773.2	26.1	1184	242	255.8	93.7	5.785	-212.16	-270.381	-270.381
	16	1848.9	1854.7	21.9	765	166	260	94.2	3.394			

6222 CONT

32	2497 8	2506 1	18	650	148	302 7	103 2	3 161	-192 784	-252 437	-252 437
33	2515 7	2521 4	13 6	51	13	302 7	103 2	0 315	-230 6	-287 459	-287 459
34	2620 9	2628 4	16 1	70	17	295 9	102 1	0 375	-188 968	-248 903	-248 903
35	2971 6	3013 4	65 2	99	22	303	103 6	3 548	-197 648	-256 942	-256 942
36	3481 9	3488 8	34 7	555	93	246 7	92 5	16 389	-445 124	-486 129	-486 129
37	3583 1	3595 4	32 4	552	92	247 5	92 9	16 337	-447 283	-488 128	-488 128
1	19 4	29 9	22 2	976	185	251 4	93 8	19 148	-440 537	-481 882	-481 882
2	99 1	109 5	21 7	974	185	250 7	93 5	19 086	-440 281	-481 644	-481 644
3	188 6	217 4	22 2	970	185	248	93	19 126	-440 416	-481 789	-481 789
4	297 4	310 2	22 8	967	183	247	93 2	18 972	-442 936	-484 103	-484 103
5*	850 8	861 5	30 7	2585	624	253 7	93 9	14 07	0	-73 9	-73 9
6	1195 1	1199 5	15 5	103	26	258 9	95 1	0 429	-131 485	-195 669	-195 669
7	1285 8	1289 9	10 9	57	13	262	96 1	0 228	-227 759	-284 828	-284 828
8	1300 6	1304 8	14 6	62	16	262 8	95 9	0 274	-114 36	-179 809	-179 809
9	1323 8	1330 9	15 9	477	96	261 6	95 7	1 935	-262 734	-317 218	-317 218
10	1399 9	1405 7	17 8	230	55	257 8	95 1	0 951	-197 465	-256 772	-256 772
11	1495 4	1502 5	17 1	161	40	260 6	93 9	0 898	-35 692	-106 655	-106 655
12	1588 2	1598 3	19 9	468	106	258 4	94 3	1 912	-172 905	-234 027	-234 027
13	1678 3	1685 4	17 6	397	90	254 3	93 8	1 195	-190 4	-250 23	-250 23
14	1764 4	1773 4	19	935	195	253 7	93	4 195	-198 961	-258 158	-258 158
36+	1765 8	1773 4	15 3	935	195	253 7	93	4 148	-199 37	-258 537	-258 537
15	1848 5	1850 1	21 5	592	129	255 7	93 6	2 518	-194 48	-254 006	-254 006
16	1927 2	1938 7	22 8	1531	303	255 9	93 7	8 125	-217 65	-275 466	-275 466
17	2005 8	2015	21 7	1031	218	261 7	94 7	4 961	-211 739	-269 991	-269 991
18	2076 4	2085 4	29 1	2200	427	262 1	94 5	13 759	-213 511	-271 633	-271 633
19	2105 5	2111 7	18	365	83	262 1	94 5	2 02	-252 789	-307 989	-307 989
20	2150	2165 9	20 3	962	204	265 8	95 3	4 823	-211 441	-269 716	-269 716
21	2212 7	2218 1	13 6	60	16	276 1	97 6	0 248	-266 604	-266 162	-266 162
22	2229 2	2243 2	24	2273	460	271 1	96 1	15 247	-207 473	-266 041	-266 041
23	2253 2	2256 8	9 2	89	14	271 1	96 1	0 4	-286 07	-338 83	-338 83
24	2262 4	2270 2	21 1	275	60	271 1	96 1	1 543	-237 752	-294 083	-294 083
25	2297 5	2307 8	18 2	793	174	271 6	96 4	3 794	-203 891	-262 816	-262 816
26	2315 7	2322 2	17 3	433	91	271 6	96 4	2 184	-260 976	-315 59	-315 59
27	2336 2	2345 6	19	106	25	277 4	97 4	0 776	-199 185	-258 366	-258 366
28	2368 5	2380 7	22 8	1990	410	273 9	96 3	12 412	-191 782	-251 509	-251 509
29	2389 3	2393 1	10 7	57	13	273 9	96 3	0 369	-255 406	-310 514	-310 514
30	2417 7	2429 2	17 6	241	53	283 7	99 2	1 195	-234 481	-291 053	-291 053
31	2435 3	2440 5	17 1	235	54	283 7	99 2	1 004	-212 67	-270 854	-270 854
32	2496 4	2505 9	18 6	497	116	277 2	97 6	2 327	-178 138	-238 874	-238 874
33	2620 9	2629	13 8	59	14	280 6	98 7	0 337	-146 478	-206 553	-206 553
34	3482 4	3509 5	33 9	923	156	245 8	92 7	27 285	-441 835	-483 083	-483 083
35	3583 1	3613 2	32 2	920	155	246 3	93	27 296	-443 024	-484 185	-484 185
1	19 4	30 9	22 2	907	153	252 7	93 8	17 761	-441 32	-482 606	-482 606
2	99 1	112 9	21 9	904	153	250 3	93 5	17 714	-441 522	-482 793	-482 793
3	198 3	210 3	22 4	903	153	249 9	92 9	17 829	-442 449	-483 652	-483 652
4	298 2	311 6	21 9	901	152	247 1	92 9	17 859	-441 685	-482 944	-482 944
5*	849	861 7	29 1	2528	603	253 8	93 9	13 462	0	-73 9	-73 9
6	1195 5	1200 1	15 5	125	30	262	96 3	0 512	-166 446	-228 046	-228 046
7	1286	1290 6	12 1	68	16	262 5	96	0 262	-171 574	-232 794	-232 794
8	1300 2	1305 2	16 3	76	19	263	96 1	0 314	-125	-189 662	-189 662
9	1324 9	1331 5	17 1	572	112	261 5	95 8	2 254	-268 7	-322 743	-322 743
10	1400 3	1406 6	18 2	277	66	257 5	94 5	1 102	-153 789	-216 324	-216 324
11	1495 8	1503 1	20 3	191	46	258 2	94 6	0 811	-167 142	-228 69	-228 69
12	1590 5	1597 2	17 3	542	122	258 4	94 9	2 224	-195 285	-254 754	-254 754
13	1678 5	1686 4	20 7	467	105	258 7	94 4	1 943	-182 477	-242 962	-242 962
14	1765 8	1774 4	24 2	1106	229	258 4	93 6	5 079	-206 527	-265 165	-265 165
36+	1765 8	1774 4	19 6	1106	229	258 4	93 6	5 017	-204 864	-263 624	-263 624
15	1848 4	1856 1	20 5	682	149	260 1	94 6	2 993	-200 37	-259 483	-259 483
16	1927 8	1939 9	23 6	1758	348	260 8	94 4	9 577	-215 724	-273 682	-273 682
17	2006 4	2016 2	20 5	1190	247	263 1	95	5 921	-213 808	-271 906	-271 906
18	2078 6	2086 7	29 5	2403	480	264 6	95 1	16 191	-214 866	-272 887	-272 887
19	2106	2112 4	17 1	447	97	264 6	95 1	2 351	-251 628	-306 933	-306 933
20	2155 8	2166 5	21 3	1124	237	269	96 3	5 888	-216 1	-274 03	-274 03
21	2213 5	2218 3	15 7	71	16	281 3	98 7	0 247	-214 833	-272 857	-272 857
22	2229 2	2244 2	24 5	2570	515	281 3	98 7	17 943	-210 573	-268 912	-268 912
23	2253 6	2257	9 2	76	16	281 3	98 7	0 396	-279 53	-332 773	-332 773
24	2262 8	2270 8	20 5	320	70	281 3	98 7	1 964	-254 11	-309 231	-309 231
25	2299 6	2308 4	16 5	918	199	271 4	97	4 508	-213 804	-271 719	-271 719
26	2316 1	2322 8	19 9	516	108	271 4	97	2 694	-275 03	-328 806	-328 806
27	2336	2346	19 4	142	31	271 4	97	1 108	-278 226	-331 567	-331 567
28	2367 8	2381 6	21 9	2245	456	276 5	97 2	14 643	-197 418	-256 729	-256 729
29	2389 7	2393 5	10 2	69	15	276 5	97 2	0 413	-285 705	-338 491	-338 491
30	2418 1	2429 6	17 3	309	68	288 7	100	1 499	-222 598	-280 048	-280 048
31	2435 5	2440 9	15 3	277	64	288 7	100	1 24	-206 096	-264 737	-264 737
32	2489 6	2506 3	18 2	572	132	283 1	98 8	2 751	-186 119	-246 295	-246 295
33	2621 7	2628 6	13 2	68	17	296 1	102	0 377	-123 876	-188 621	-188 621
34	3483 4	3492	33 4	964	145	250 3	93 4	25 533	-442 398	-483 605	-483 605
35	3583 1	3608 6	31 8	862	146	249	93 2	25 576	-442 165	-483 389	-483 389

Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs. VSMOW
Duplicate 1											
1	19.4	20.5	21.7	509	81	33.1	25.9	9.703	-449.79	-490.45	-490.45
2	99.1	100.1	21.7	505	80	33.1	25.3	9.633	-444.774	-485.805	-485.805
3	198.6	199.6	21.9	504	80	33.1	25.4	9.608	-445.689	-486.653	-486.653
4	298	299.1	21.9	502	78	33.1	25.8	9.462	-448.982	-489.702	-489.702
5	509.8	529.6	99.7	2589	731	40.6	27.7	54.841	-23.543	-95.703	-95.703
6*	1140.9	1167.5	73.6	1825	518	55.5	32	40.985	0	-73.9	-73.9
7	1279.7	1299.8	65	170	42	64.3	33.7	4.176	-134.508	-198.468	-198.468
8	1429.8	1455.7	70.4	199	44	76.7	36.7	5.243	-219.109	-276.817	-276.817
9	1574.8	1611.2	81.5	439	101	73.3	35.9	10.822	-177.327	-238.123	-238.123
10	1685.6	1710.5	55	104	21	100.3	41.1	2.319	-278.558	-331.872	-331.872
11	1741.8	1774.8	72.7	234	53	96.5	40.5	5.785	-201.864	-260.846	-260.846
12	1816.8	1849.7	97	838	127	83.5	37.8	15.785	-284.354	-337.24	-337.24
13	1914.9	1941.4	75.9	554	125	70.4	34.8	13.071	-186.373	-246.5	-246.5
14	2077.5	2105	107.2	386	89	60.8	32	11.005	-168.707	-230.14	-230.14
15	2236.3	2282.1	92	1473	328	58.6	31.2	45.735	-205.325	-264.051	-264.051 C23
16	2356.7	2435.5	156.5	778	175	107.8	42.4	35.469	-210.987	-269.295	-269.295
17	2549	2599.1	118.9	1774	397	61.2	31.8	58.262	-202.798	-261.711	-261.711 C25
18	2701.3	2737.3	84.2	785	176	75.8	35.3	21.822	-192.971	-252.611	-252.611
19	2843	2908	125.4	2518	575	87.7	37.5	104.319	-200.045	-259.162	-259.162 C27
20	2990.8	3033.8	129.6	1070	238	155.2	53.6	30.192	-198.799	-258.008	-258.008
21	3121.2	3203.6	146.9	3361	777	114	44.6	170.508	-206.614	-265.245	-265.245 C29
22	3266.1	3308.3	113.5	1032	228	114	44.6	32.076	-204.024	-262.846	-262.846
23	3383.1	3451	118.5	2005	461	129.7	47.9	81.471	-192.92	-252.563	-252.563
24	3502	3520	32.2	141	28	350	98.3	1.379	-385.759	-431.151	-431.151
25	3534.2	3546.3	34.7	70	15	350	98.3	-1.76	-231.185	-288.001	-288.001
26	3569.7	3589.6	48.1	89	18	184.7	61.3	1.124	-372.771	-419.123	-419.123
27	3618.6	3673.2	93	934	216	157	53.7	27.085	-168.759	-230.187	-230.187
28	3711.6	3720	25.7	78	19	157	53.7	1.392	-154.651	-217.122	-217.122
29	3757.8	3780.8	59.6	279	61	153.4	53.1	5.826	-205.532	-264.243	-264.243
30	3850.4	3883	51	207	48	107.8	43.1	4.746	-178.809	-239.495	-239.495
31*	3962	4017	117	1577	359	161.7	56	49.597	0	-244.1	-244.1
32	4996.1	4997	101.4	328	51	45.8	29.7	30.475	-333.856	-496.461	-496.461
33	5115.5	5116.5	61.7	327	52	33.2	25.4	18.811	-306.589	-475.851	-475.851
Duplicate 2											
1	19.4	20.5	21.7	315	50	33.2	25.5	6.021	-443.315	-484.454	-484.454
2	99.1	100.1	21.7	312	51	33.3	25.7	5.98	-444.888	-485.91	-485.91
3	198.6	199.6	21.9	310	51	33.3	25.4	5.962	-440.845	-482.186	-482.186
4	298	299.1	21.7	309	50	33.3	25.4	5.878	-440.98	-482.291	-482.291
5	510.6	530.7	99.3	2632	744	40.8	27.5	55.779	-26.454	-98.399	-98.399
6*	1141.6	1168.3	73.6	1841	523	57.2	31.9	41.418	0	-73.9	-73.9
7	1280.5	1300.6	65	185	44	66.3	34.2	4.491	-140.511	-204.027	-204.027
8	1430.8	1456.7	70.2	215	47	79.8	37.4	5.626	-221.789	-279.299	-279.299
9	1575.9	1612.4	81.7	477	109	76.1	36.6	11.609	-183.123	-243.49	-243.49
10	1686.6	1711.5	55.2	114	23	104.8	42.5	2.516	-316.887	-367.369	-367.369
11	1743.1	1776.1	72.9	254	58	100.6	41.2	6.221	-198.119	-257.378	-257.378
12	1817.7	1851.3	97.4	685	136	86.6	38.6	16.979	-289.112	-341.646	-341.646
13	1915.9	1942.9	75.7	604	137	73	35.2	13.979	-187.126	-247.197	-247.197
14	2078.3	2106.3	108.1	424	97	62.5	32.8	11.748	-189.071	-248.999	-248.999
15	2236.9	2284.2	93.2	1554	345	60.3	31.8	48.839	-212.294	-270.44	-270.44 C23
16	2358.4	2437.8	155.7	834	188	112.2	43.2	37.86	-214.284	-272.33	-272.33
17	2549.6	2601.4	120.4	1850	414	63.4	32	62.048	-208.728	-265.35	-265.35 C25
18	2702.4	2739.6	85.3	829	185	79.4	36.2	23.168	-199.192	-258.371	-258.371
19	2843.7	2910.7	127.5	2608	597	92.5	38.9	110.378	-207.088	-265.684	-265.684 C27
20	2992	3036.8	128.5	1097	244	166	56.3	31.637	-207.746	-266.293	-266.293
21	3121.6	3206.9	148	3450	799	121.7	46.5	179.719	-211.982	-270.216	-270.216 C29
22	3269.6	3311	112	1068	236	121.7	46.5	33.906	-211.964	-270.2	-270.2
23	3383.7	3454.1	121.2	2073	477	135.8	49.4	86.574	-200.396	-259.487	-259.487
24	3504.9	3523.1	31.8	374	81	135.8	49.4	8.793	-242.007	-298.023	-298.023
25	3536.7	3548.8	34.7	305	69	135.8	49.4	6.259	-207.689	-266.24	-266.24
26	3572.2	3592.3	47.9	90	20	195.2	62.2	1.125	-166.182	-227.801	-227.801
27	3620.7	3675.7	93.4	974	224	165	55.5	28.692	-177.067	-237.882	-237.882
28	3714.1	3722.3	25.3	82	20	165	55.5	1.427	-164.268	-226.028	-226.028
29	3760.1	3783.3	58.9	286	63	160.6	54.7	6.054	-212.863	-271.033	-271.033
30	3851.7	3885.1	51.6	216	51	111.7	43.6	5.023	-174.835	-235.815	-235.815
31*	3962.8	4017.8	121.2	1532	350	168	56.4	46.941	0	-244.1	-244.1
32	4996.1	4997	101.2	210	33	45.6	29.3	18.994	-326.93	-491.226	-491.226
33	5115.5	5116.5	61.7	206	34	33.2	25.5	11.978	-294.523	-466.73	-466.73

1022

Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (V/s)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs. VSMOW
Duplicate 1											
1	19.4	20.3	21.7	786	124	28.5	22.3	14 887	-451 078	-491 642	-491 642
2	99.1	99.9	21.7	794	124	28.5	22.3	14 87	-451 773	-492 287	-492 287
3	198.6	199.6	21.9	781	123	28.5	22.4	14 934	-452 35	-492 821	-492 821
4	298	299.1	21.7	785	124	28.5	22.6	14 832	-451 979	-492 478	-492 478
5	443.3	455	87.6	970	265	22.6	22.6	17 194	-31 536	-103 105	-103 105
6*	1075.3	1065.6	89.9	1421	394	34.4	23.8	27 123	0	-73.9	-73.9
7	1628.1	1635	42	67	18	37.3	24.3	1 027	-166 378	-227 983	-227 983
8	1724	1731.6	28.8	73	17	35.5	23.9	1 008	-166 785	-228 36	-228 36
9	1816.6	1827.3	54.5	277	62	35.5	23.4	4 486	-182 925	-243 307	-243 307
10	1902.9	1914	30.7	131	29	41.2	25	1 732	-197 72	-257 009	-257 009
11	1933.7	1940.6	48.7	116	27	41.2	25	1 812	-171 373	-232 608	-232 608
12	1991.1	2004.1	63.7	522	112	39.4	24.7	8 842	-210 357	-268 712	-268 712
13	2074.1	2084.6	43.9	303	66	39.5	24.4	4 636	-195 419	-254 877	-254 877
14	2152.5	2171.9	79	1182	255	40	24.8	22 149	-212 481	-270 879	-270 879
15	2231.9	2243.2	71.5	405	87	50.9	27.2	6 293	-211 883	-270 125	-270 125
16	2304.6	2326.3	59.6	1621	397	44.6	25.2	36 579	-214 954	-272.7	-272.7
17	2364.2	2369	18.1	135	32	44.6	25.2	1 845	-185 971	-227 605	-227 605
18	2380.3	2391.2	56.4	512	111	44.6	25.2	8 923	-206 481	-265 122	-265 122
19	2449.3	2459.7	46.2	362	78	59.3	29.1	5 866	-221 195	-278 748	-278 748
20	2513.4	2522.8	42	200	43	65.1	30.2	2 781	-224 708	-282 002	-282 002
21	2558	2567.4	24	89	19	62.9	29.7	1 004	-243 115	-299 049	-299 049
22	2582	2586.9	18.2	68	15	62.9	29.7	0 806	-216 785	-274 684	-274 684
23	2644.5	2651.2	19	59	14	55.3	28.1	0 849	-183 062	-243 452	-243 452
24*	2789.5	2802.7	99.9	2049	461	58.9	28.7	49 543	0	-244.1	-244.1
25	3482.8	3483.8	31.8	748	118	28.7	22.5	21 36	-314 529	-481 853	-481 853
26	3582.3	3583.3	32	752	118	28.4	22.1	21 413	-312 303	-480 17	-480 17
Duplicate 2											
1	19.4	20.3	21.7	749	117	28.5	22.3	14 117	-452 459	-492 923	-492 923
2	99.1	99.9	21.7	751	118	28.5	22	14 091	-451 34	-491 886	-491 886
3	198.6	199.4	21.9	744	118	28.5	22.1	14 173	-451.2	-491 756	-491 756
4	298	299.1	21.7	743	117	28.5	22.2	14 085	-452 212	-492 894	-492 894
5	442.9	455.8	80.3	1087	297	29.7	22.2	19 33	-31 929	-103 469	-103 469
6*	1075.7	1065.6	91.1	1500	418	34.6	23.5	29 296	0	-73.9	-73.9
7	1627.5	1635.2	42.2	68	16	37.6	24.1	1 033	-131 369	-195 581	-195 581
8	1723.2	1731.8	29.5	74	17	35.7	23.9	1 014	-180 103	-240 893	-240 893
9	1815	1827.3	56.6	280	61	35.6	23.5	4 555	-190 962	-250 749	-250 749
10	1903.2	1914.2	30.3	29	25	41.5	25	1 731	-199 495	-258 652	-258 652
11	1933.5	1940.8	48.5	116	28	41.5	25	1 837	-188 305	-248 289	-248 289
12	1989.7	2004.3	85.4	521	113	39.9	24.8	8 76	-213 082	-271 235	-271 235
13	2072.9	2084.8	45.4	303	67	40	24.2	4 693	-192 434	-252 113	-252 113
14	2151.7	2171.9	78.4	1179	258	40.4	24.6	22 512	-210 545	-268 886	-268 886
15	2230.7	2243.4	72.1	405	87	52.7	27.8	6 327	-228 543	-285 553	-285 553
16	2303.6	2326.3	61.2	1806	395	45.6	25.8	37 225	-215 311	-273.3	-273.3
17	2364.8	2391.4	71.9	514	110	45.6	25.8	10 626	-211 047	-269 35	-269 35
18	2447.4	2459.7	48.5	359	78	62.4	29.5	5 84	-216 429	-274 334	-274 334
19	2512.2	2522.8	43.3	198	43	67.7	30.7	2 898	-230 979	-287 809	-287 809
20	2557.1	2567.4	24.9	89	19	63.5	29.8	1 023	-285 293	-314 957	-314 957
21	2582	2589.1	18.4	68	15	63.5	29.8	0 813	-230 648	-287 503	-287 503
22	2644.1	2651.4	19.6	63	15	63.5	29.8	0 701	-180 897	-241 428	-241 428
23	2683.7	2699.8	34.3	52	12	56	28	0 809	-183 354	-243 704	-243 704
24*	2789.4	2803.1	101.4	2114	477	61.4	29.6	53 09	0	-244.1	-244.1
25	3482.8	3483.8	31.8	711	112	28.8	22.1	20 261	-310 454	-478 772	-478 772
26	3582.3	3583.3	32	714	112	28.4	22	20 322	-309 601	-478 127	-478 127
Duplicate 3											
1	19.4	20.5	21.7	626	100	33.2	25.2	11 976	-448 97	-487 839	-487 839
2	99.1	99.9	21.9	622	99	33.2	25.2	11 995	-445 408	-486 392	-486 392
3	198.6	199.6	21.9	621	99	33.2	25.3	11 944	-447 051	-487 914	-487 914
4	298	299.1	21.9	621	98	33.3	25.4	11 825	-447 382	-488 22	-488 22
5	442.9	455.8	80.3	1087	297	29.7	22.2	19 33	-31 929	-103 469	-103 469
6*	1075.7	1065.6	91.1	1500	418	34.6	23.5	29 296	0	-73.9	-73.9
7	1282.2	1297.7	62.9	78	17	60.6	32.9	2 37	-160 536	-222 572	-222 572
8	1416.4	1449.6	66.7	92	23	62.5	32.7	2 311	-116 212	-181 524	-181 524
9	1585.1	1603.4	38.2	155	36	64.1	33.5	3 009	-195 039	-254 526	-254 526
10	1737.2	1766.5	68.8	144	33	63.5	32.9	3 296	-188 62	-248 581	-248 581
11	1815.6	1835.6	52.3	89	18	63.2	32.9	1 87	-274 747	-328 343	-328 343
12	1910.9	1933.5	77.7	337	76	54.1	30.3	8 369	-179 712	-240 332	-240 332
13	2073.9	2088.8	55	342	77	52.4	30.3	8 574	-199 573	-258 725	-258 725
14	2233.8	2271.6	112.4	1185	259	48.2	28.8	34 595	-209 193	-267 634	-267 634
15	2398.7	2427.5	109.5	833	142	79.2	36.2	25 173	-205 021	-263 77	-263 77
16	2545.6	2598	119.5	1932	426	51.3	29.3	65 202	-212 446	-270 846	-270 846
17	2697.1	2738.1	142.5	871	219	60.4	31.3	36 88	-204 206	-263 015	-263 015
18	2841.4	2917.6	148.6	3543	813	66.1	32.5	162 434	-213 082	-271 235	-271 235
19	2990.8	3038.9	129.8	1233	273	88.9	38.2	48 066	-216 408	-274 316	-274 316
20	3122.3	3224.2	156.5	4049	1163	70.9	33.8	283 54	-215 519	-273 492	-273 492
21	3278.8	3326.7	95.7	1798	394	70.9	33.8	63 44	-218 777	-276 509	-276 509
22	3399.4	3448.9	88.2	1417	311	127.5	46.5	44 682	-216 793	-274 672	-274 672
23	3488.6	3523.9	49.1	286	57	254.6	76.5	5 241	-302 176	-363 745	-363 745
24	3537.7	3555.1	42.8	420	89	254.6	76.5	8 467	-253 656	-308 811	-308 811
25	3580.6	3602.7	47.2	270	51	254.6	76.5	3 561	-383 586	-429 148	-429 148
26	3646	3659	31.6	141	33	213.2	64.6	1 347	-68 887	-137 696	-137 696
27	3753.4	3777	58.3	260	57	103	41	6 317	-223 63	-281 004	-281 004
28	3846.2	3875.3	46.8	108	25	103.1	41	2 152	-160 199	-250 044	-250 044
29	3996.6	4030.8	123.1	2650	610	113.1	43	104 058	0	-244.1	-244.1
30	4134.6	4150.1	53.7	50	12	114.6	43.3	1 196	65 305	-194 736	-194 736
31	4995.9	4997	101.6	508	79	41.1	27.4	47 865	-316 269	-483 168	-483 168
32	5115.5	5116.3	61.7	504	79	33.3	25.8	29 036	-314 195	-481 6	-481 6
Duplicate 4											
1	19.4	20.5	21.7	494	79	33.3	25.1	9 436	-444 704	-485 74	-485 74
2	99.1	100.1	21.7	491	78	33.4	25.5	9 403	-448 083	-488 87	-488 87
3	198.6	199.6	21.9	492	78	33.4	25	9 42	-444 508	-485 559	-485 559
4	298	299.1	21.9	492	78	33.4	25	9 321	-444 282	-485 349	-485 349
5	508.3	527.5	98.6	1979	557	37.8	26.3	42 873	-24 163	-96 278	-96 278
6*	1141.8	1162.9	125.4	5038	1500	58.4	32.4	147 81	0	-73.9	-73.9
7	1283.1	1300	63.5	78	18	62.6	33.4	2 553	-150 02	-212 834	-212 834
8	1417	1451.1	88.1	93	22	64.9	34.1	2 479	-200 349	-259 444	-259 444
9	1570.8	1606.8	87.8	149	35	61.6	32.5	4 813	-133 679	-197.7	-197.7
10	1737.6	1789.8	69.8	131	30	67.4	34	3 431	-194 322	-253 861	-253 861
11	1815.2	1839	53.5	79	18	65.9	33.3	1 976	-246 716	-302 383	-302 383
12	1910.5	1936.8	66.7	301	68	57.1	31.4	8 901	-188 864	-248 807	-248 807
13	2072.9	2102.3	56.8	307	70	54.3	30.9	9 099	-200 256	-259 357	-259 357
14	2233	2273.3	113.5	1150	258	49.9	29	36 972	-205 695	-264 58	-264 58
15	2397.2	2430.7	112.7	663	150	88.1	38.1	26 366	-201 124	-260 161	-260 161
16	2544.6	2596.2	120.4	2049	455	53.4	29.8	69 592	-212 14	-270 363	-270 363
17	2696.1	2737.3	1								

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22	3358 4	3365 9	32	151	35	69 9	33 6	3 121	-197 32	-256 638	-256 638
23	3390 4	3435 3	86 1	1387	307	89 9	33 6	53 405	-217 113	-274 956	-274 956
24	3478 9	3508 1	52 5	364	76	225 1	70	9 404	-271 864	-325 673	-325 673
25	3529 4	3544 6	32 6	411	87	225 1	70	8 838	-239 569	-295 764	-295 764
26	3582	3588 5	55	312	61	225 1	70	6 405	-319 997	-370 249	-370 249
27	3638 9	3651 6	32 2	127	29	206 6	64 2	1 228	-124 75	-189 431	-189 431
28	3739 8	3767 6	66 7	258	56	127 1	46 5	5 374	-216 669	-276 428	-276 428
29	3842	3871 5	48 3	100	23	107 6	42	2 215	-187 938	-247 949	-247 949
30*	3957	4027 6	131	2583	595	126 3	46 3	106 794	0	-244 1	-244 1
31	4132 8	4148 9	53 9	52	12	114	43 7	1 246	-0 154	-244 217	-244 217
32	4606 1	4997	101 4	405	62	42	28 3	37 76	-323 839	-488 89	-488 89
33	5115 5	5116 5	61 7	397	64	33 3	25 3	23 028	-306 887	-476 076	-476 076

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Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs. VSMOW	
Duplicate 1												
1	19.4	20.3	21.9	1014	165	33.3	25.3	19.345	-443.392	-484.525	-484.525	
2	99.1	99.9	21.9	1004	163	33.4	25.2	19.187	-443.324	-484.462	-484.462	
3	198.6	199.6	21.9	999	162	33.4	25	19.132	-442.898	-484.068	-484.068	
4	298	299.1	21.9	998	161	33.4	25.1	18.835	-443.292	-484.432	-484.432	
5	506	526.3	98	2465	699	38.1	26.7	52.187	-26.887	-98.8	-98.8	
6	782.3	794	58.8	136	34	36.4	26.1	2.675	-120.076	-185.102	-185.102	
7*	1144.5	1170.2	95.3	1813	516	46.6	29	40.506	0	-73.9	-73.9	
8	1284.7	1303.3	81.4	85	20	52.5	30.4	2.253	-161.6	-223.558	-223.558	
9	1420.4	1453.8	65.4	107	26	59.4	32.1	2.735	-167.16	-228.707	-228.707	
10	1528.8	1552.7	59.1	156	30	63.9	33.1	3.931	-324.52	-374.438	-374.438	
11	1590.7	1615.8	62.7	504	113	78.3	35.8	12.341	-203.929	-262.758	-262.758	
12	1695	1717.1	48.1	78	16	74.7	35	1.893	-292.13	-344.442	-344.442	
13	1743.9	1778	78.4	280	62	82.1	36.6	8.369	-244.694	-300.511	-300.511	
14	1823.9	1853	55.8	522	103	77	35.7	12.574	-301.484	-353.104	-353.104	
15	1879.7	1892.9	40.3	121	29	77	35.7	2.788	-186.001	-246.156	-246.156	
16	1920.1	1945.8	76.3	518	117	77	35.7	12.809	-195.664	-255.105	-255.105	
17	2081.4	2110.5	61	400	92	52.3	29.7	11.241	-195.348	-254.812	-254.812	
18	2240.7	2285.6	119.1	1625	362	47.2	28.3	50.575	-208.671	-267.335	-267.335	
19	2401.2	2435.1	99.3	643	146	58.4	30.7	18.885	-196.764	-256.123	-256.123	
20	2553.1	2605.8	118.1	1845	412	50.1	29	61.417	-213.547	-271.066	-271.066	
21	2706.3	2740.8	81.5	666	151	68	33.4	20.979	-204.063	-262.863	-262.863	
22	2848.9	2898.6	142.7	1683	379	68.3	32.8	61.502	-204.963	-263.744	-263.744	
23	2962.5	3032.8	108.5	769	176	100.8	41.1	28.373	-202.289	-261.24	-261.24	
24	3124.8	3205.2	120	3114	731	72.7	34.1	163.619	-200.307	-259.404	-259.404	
25	3244.7	3258.9	33.6	898	197	72.7	34.1	22.098	-231.752	-288.526	-288.526	
26	3278.4	3310.6	104.5	1212	277	72.7	34.1	45.15	-197.81	-257.091	-257.091	
27	3385.8	3468.4	129.8	2713	639	113.9	43.6	148.235	-194.237	-253.783	-253.783	
28	3518.2	3542.1	49.3	155	28	490.9	131.5	1.988	-542.108	-575.946	-575.946	
29	3565.5	3652.5	180.2	2692	584	490.9	131.5	215.340	-219.707	-277.37	-277.37	
30	3773.9	3815.9	96.8	1134	245	176	58.9	36.01	-228.539	-285.55	-285.55	
31	3871.3	3914.2	109.3	1699	411	128.7	47.9	55.462	-143.526	-206.819	-206.819	
32*	3981	4029.1	107	2041	470	138.4	51.5	64.928	0	-244.1	-244.1	
33	4069.1	4102.9	29.6	117	28	108.2	45.4	1.779	41.321	-212.965	-212.965	
34	4996.1	4997	101.4	636	99	53.6	32.4	59.353	-335.639	-497.811	-497.811	
35	5115.5	5116.5	61.9	639	101	33.4	25.3	36.383	-312.632	-480.419	-480.419	
Duplicate 2												
1	19.4	20.5	21.7	609	97	33.3	25.5	11.613	-451.243	-491.796	-491.796	
2	99.1	100.1	21.7	603	96	33.3	25.2	11.53	-449.031	-489.748	-489.748	
3	198.6	199.6	21.9	601	96	33.4	25.5	11.488	-450.523	-491.129	-491.129	
4	298	299.1	21.9	600	94	33.4	25.5	11.322	-450.812	-491.397	-491.397	
5	506.6	527.3	99.3	2676	760	38.5	26.6	57.096	-28.036	-99.864	-99.864	
6	782.9	794.4	56.2	150	37	36.7	26.3	2.886	-131.191	-195.396	-195.396	
7*	1144.9	1171.2	96.3	1955	558	47.1	29	44.076	0	-73.9	-73.9	
8	1285.6	1301.7	58.5	99	23	54.1	30.8	2.349	-171.948	-233.141	-233.141	
9	1421.8	1451.7	62.7	126	30	60.9	32.5	2.887	-170.909	-232.179	-232.179	
10	1529	1550.8	54.5	195	38	64.4	32.8	4.183	-307.242	-358.437	-358.437	
11	1562.8	1615.8	60.4	618	137	80.5	36.2	13.044	-206.368	-265.017	-265.017	
12	1693.1	1714.8	51.2	101	20	75.5	35.6	2.113	-335.264	-384.388	-384.388	
13	1745.4	1777.8	78.4	345	76	79.2	35.6	9.26	-236.685	-293.094	-293.094	
14	1825.8	1853.8	55.6	631	124	76	35.2	13.587	-297.999	-349.877	-349.877	
15	1861.4	1891.7	41.2	189	40	76	35.2	3.112	-171.562	-232.811	-232.811	
16	1923.2	1948.2	71.3	662	146	71.3	35	14.017	-210.099	-268.473	-268.473	
17	2085.2	2109.9	56.4	549	123	51.7	29.7	11.993	-199.746	-258.885	-258.885	
18	2245.1	2289.2	112.9	1777	396	47.1	28.1	53.676	-208.264	-266.774	-266.774	
19	2406.2	2436.1	99.3	843	185	59.2	31.2	20.218	-202.628	-261.832	-261.832	
20	2557.7	2606.9	108.7	2001	445	49.9	29.1	65.179	-214.604	-272.644	-272.644	
21	2710.7	2742.3	76.8	901	198	65.4	32.2	22.81	-198.975	-258.171	-258.171	
22	2853.7	2902.4	116	1892	424	66.2	32.4	64.436	-207.247	-265.832	-265.832	
23	2968.3	3034.9	95.7	1148	256	93.8	38.9	31.247	-197.606	-257.088	-257.088	
24	3131.4	3212.5	122.1	3435	797	75.1	34.6	177.678	-201.315	-260.338	-260.338	
25	3283	3314.3	96.1	1287	284	286.9	85.9	25.813	-220.254	-277.877	-277.877	
26	3386.2	3473.4	128.3	2883	672	122	45.4	150.241	-194.278	-253.821	-253.821	
27	3514.5	3535.9	54.5	624	136	122	45.4	22.777	-231.163	-287.98	-287.98	
28	3569.1	3659.4	180.2	3232	701	122	45.4	292.993	-222.638	-280.085	-280.085	
29	3780.6	3822.2	95.3	1205	259	173.8	58.1	36.812	-225.688	-282.91	-282.91	
30	3875.9	3918.3	109.5	1693	411	173.8	58.1	52.286	-132.763	-196.851	-196.851	
31*	3985.8	4035.6	107.8	2169	500	145.8	53.3	70.962	0	-244.1	-244.1	
32	4094.3	4107.9	29.1	117	28	118.1	48.2	1.756	24.752	-225.39	-225.39	
33	4996.1	4997.2	101.4	391	60	55.3	32.6	35.729	-349.87	-508.567	-508.567	
34	5115.7	5116.5	61.7	394	62	33.4	25.2	22.435	-309.677	-478.185	-478.185	

Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs.
Duplicate 1											
1	19.4	20.5	21.7	147	26	33.1	25.2	2.833	-403.485	-447.568	-447.568
2	99.1	100.1	21.7	146	26	33.1	25.2	2.814	-400.377	-444.689	-444.689
3	198.6	199.6	21.7	146	25	33.1	25.5	2.81	-414.323	-457.604	-457.604
4	298.2	299.1	21.5	145	25	33.1	25.4	2.771	-407.773	-451.538	-451.538
5	509.3	529.6	99.9	2691	761	40.4	27.6	57.325	-36.544	-107.744	-107.744
6*	1139.3	1165.2	95.5	1850	529	38.3	26.6	41.834	0	-73.9	-73.9
7	1427.9	1441.1	45.6	52	14	45.9	28.6	1.067	-69.437	-138.205	-138.205
8	1584.8	1600.3	33.6	125	30	52.8	30.4	2.014	-141.813	-205.233	-205.233
9	1736	1764.2	69.6	143	34	57.1	31.8	3.043	-196.954	-256.299	-256.299
10	1809.1	1835.2	60.6	175	36	57.4	31.8	3.351	-280.514	-333.684	-333.684
11	1911.7	1929.9	64.8	222	52	53	30.2	4.448	-144.106	-207.357	-207.357
12	2074.5	2094.6	56.2	259	59	51.3	30	5.049	-167.894	-229.387	-229.387
13	2234.2	2265.4	80.3	762	168	50.6	29.6	18.327	-203.863	-262.697	-262.697
14	2393.3	2416	73.1	337	76	54.2	30.5	6.678	-173.399	-234.485	-234.485
15	2544.2	2577.6	82.6	758	167	50.7	29.8	18.501	-203.148	-262.035	-262.035
16	2694.6	2719.9	76.1	376	86	53.1	30.1	8.032	-174.777	-235.761	-235.761
17	2838.4	2871	82.3	731	163	52.6	29.7	18.105	-186.666	-246.799	-246.799
18	2979.9	3006	76.5	421	95	56.6	30.2	9.207	-171.055	-232.314	-232.314
19	3113.9	3152.6	74.4	972	217	54.2	30.2	25.979	-191.169	-250.942	-250.942
20	3188.9	3204.8	58.1	58	12	149.1	53.2	-0.892	59.902	-18.425	-18.425
21	3248.3	3272.9	62.3	370	83	65.4	33	7.701	-188.167	-248.161	-248.161
22	3367.8	3406.1	86.5	625	142	63.3	32	16.184	-181.737	-242.207	-242.207
23	3456.7	3480.9	47.9	102	22	80.9	36.6	1.946	-257.408	-312.286	-312.286
24	3505.1	3520.8	36.4	130	31	82.8	36.6	2.106	-181.85	-232.789	-232.789
25	3543	3564.7	48.9	171	35	102	41.7	3.103	-285.683	-338.471	-338.471
26	3621.6	3639.9	64.8	194	45	93.3	39	3.073	-139.631	-203.212	-203.212
27	3716.2	3753.2	83	206	46	65	32.7	4.764	-196.917	-256.264	-256.264
28	3833.3	3863.6	52	53	13	60.3	31.8	1.292	-138.857	-202.496	-202.496
29*	3950.9	4004.9	116.6	1603	365	66	34.1	53.156	0	-244.1	-244.1
30	4995.7	4996.8	101.2	99	17	42.8	28.4	8.882	-271.223	-449.117	-449.117
31	5115.3	5116.1	61.4	100	19	33.1	25.5	5.819	-224.348	-413.684	-413.684
Duplicate 2											
1	19.4	20.5	21.5	96	18	33.2	25.4	1.866	-378.948	-424.843	-424.843
2	99.1	100.1	21.5	96	18	33.2	25.3	1.852	-377.29	-423.308	-423.308
3	198.6	199.6	21.7	95	18	33.3	25.6	1.851	-387.241	-432.524	-432.524
4	298	299.1	21.5	94	19	33.3	25.3	1.826	-371.735	-418.163	-418.163
5	508.9	529.6	99.9	2915	828	41	27.3	62.19	-36.31	-107.527	-107.527
6*	1139.7	1167.9	100.9	2095	597	38.7	26.2	47.689	0	-73.9	-73.9
7	1430.6	1442.1	44.5	53	14	46.2	28.8	1.086	-88.817	-156.153	-156.153
8	1588.4	1601.1	30.7	131	32	52.9	30.4	2.026	-143.689	-206.971	-206.971
9	1753.5	1765.2	52.9	124	30	85.3	37.3	1.369	-62.728	-131.993	-131.993
10	1818.1	1836.3	53.1	186	39	58.8	31.1	3.381	-233.549	-290.004	-290.004
11	1915.1	1931.4	63.7	237	55	52.7	30.5	4.646	-169.891	-231.236	-231.236
12	2078.5	2096.3	53.7	278	63	51.3	30	5.262	-173.09	-234.199	-234.199
13	2237.6	2268.1	78	826	180	51	30.1	19.16	-211.564	-269.829	-269.829
14	2397.4	2418.1	71.5	366	83	54.6	30.2	7.28	-165.942	-227.578	-227.578
15	2547.3	2580.5	80.9	832	182	51.5	30.1	19.613	-206.781	-285.4	-285.4
16	2697.1	2722.2	75.9	415	94	54.1	30.4	8.625	-178.89	-237.718	-237.718
17	2842	2874.2	79.8	811	179	53.6	30.3	19.575	-194.57	-254.091	-254.091
18	2984.1	3008.6	73.8	475	107	57.7	31.2	10.071	-178.103	-238.842	-238.842
19	3116.8	3156.5	73.4	1090	242	55.7	30.7	28.337	-192.36	-252.044	-252.044
20	3190.6	3206.3	60.8	61	12	168.4	57.9	-1.48	12.587	-82.244	-82.244
21	3253.7	3276.1	85.7	427	95	66.7	33.4	9.075	-193.062	-252.694	-252.694
22	3371.2	3410.3	89	716	161	64.4	32.2	18.261	-181.419	-241.912	-241.912
23	3462.1	3484	47.2	124	26	83.7	37.5	2.285	-268.986	-323.008	-323.008
24	3509.3	3523.9	38.5	164	37	83.7	37.5	2.611	-199.972	-259.094	-259.094
25	3548.6	3568	47	217	45	103.9	42	3.746	-269.256	-323.258	-323.258
26	3596.3	3608.6	28.6	53	13	99.9	40.4	0.664	-208.348	-268.851	-268.851
27	3625.3	3642.7	64	240	55	94.5	39.2	3.85	-140.457	-203.978	-203.978
28	3718.5	3755.9	83.2	262	58	68.2	33.2	5.613	-186.774	-246.872	-246.872
29	3836.4	3865.2	51	66	16	63	32.4	1.532	-143.45	-206.749	-206.749
30*	3952	4014.7	127.1	2004	456	68.8	34.1	70.563	0	-244.1	-244.1
31	4995.7	4996.8	101.2	65	13	42.9	28.5	5.626	-254.223	-436.267	-436.267
32	5115.1	5116.1	61.4	66	13	33.1	25.2	3.884	-156.242	-362.203	-362.203
Triplicate 1											
1	19.4	27.8	21.7	874	146	253.2	94.2	17.135	-444.875	-485.898	-485.898
2	99.1	105.3	21.7	872	146	254.1	94.2	17.076	-444.266	-485.335	-485.335
3	197.9	211.5	23	870	145	252.6	94.3	17.272	-445.238	-486.235	-486.235
4	298	302.6	22.2	867	144	254.4	94.8	17.005	-446.186	-487.113	-487.113
5*	872.2	892.8	45.6	6737	1673	258.8	95.7	69.529	0	-73.9	-73.9
6	991.3	1002.6	48.1	244	64	292	104.6	5.743	-107.386	-173.351	-173.351
7	1103.1	1121.1	43.1	641	165	376.8	127.8	12.723	-128.844	-193.223	-193.223
8	1146.2	1234.4	121	1559	390	376.8	127.8	49.075	-135.718	-199.589	-199.589
9	1267.2	1343.7	87.2	1829	457	376.8	127.8	81.321	-179.863	-240.471	-240.471
10	1354.3	1373.3	38	2460	537	376.8	127.8	49.241	-260.1	-314.779	-314.779
11	1392.4	1445.9	76.3	2964	731	376.8	127.8	74.137	-159.264	-221.395	-221.395
12	1468.6	1541.8	97.2	3094	777	376.8	127.8	86.949	-163.88	-225.669	-225.669
13	1565.8	1568.2	50	463	112	376.8	127.8	15.702	-144.983	-208.169	-208.169
14	1615.8	1655.3	51.2	10522	2632	376.8	127.8	231.164	-215.127	-273.129	-273.129
15	1667	1735.1	94.5	4750	1143	376.8	127.8	115.61	-181.657	-242.133	-242.133
16	1781.5	1835	86.3	10479	2579	376.8	127.8	244.609	-209.59	-268.002	-268.002
17	1847.8	1908.2	78.8	5310	1307	376.8	127.8	123.937	-184.544	-244.806	-244.806
18	1926.6	2002.4	115.2	10198	2547	376.8	127.8	276.48	-203.731	-262.575	-262.575
19	2041.7	2072.7	67.9	5180	1307	376.8	127.8	143.708	-190.694	-250.502	-250.502
20	2109.6	2171.7	65.2	15057	3946	376.8	127.8	375.347	-208.264	-266.773	-266.773
21	2181.3	2183.6	5.2	132	23	2884.7	722.9	0.189	-791.497	-806.906	-806.906
22	2201.2	2230	58.1	5431	1347	1032.7	283.4	103.847	-181.39	-241.886	-241.886
23	2260.5	2315.9	65.4	9689	2441	968.9	269.2	223.131	-191.083	-250.862	-250.862
24	2326	2341.2	31.1	1708	389	968.9	269.2	39.619	-243.152	-299.083	-299.083
25	2357.1	2373.2	21.5	4621	1068	968.9	269.2	46.301	-198.71	-257.926	-257.926
26	2378.6	2399.3	26.8	4346	964	968.9	269.2	69.521	-246.624	-302.299	-302.299
27	2405.4	2417.3	14.6	2634	575	968.9	269.2	21.678	-233.192	-289.859	-289.859
28	2420	2439.4	25.7	4974	1169	968.9	269.2	64.273	-183.09	-243.46	-243.46
29	2445.7	2448	11.1	227	53	968.9	269.2	0.484	-298.123	-349.992	-349.992
30	2470.6	2492.1	42	3650	884	915.2	253.6	62.211	-224.658	-281.956	-281.956
31	2518	2523.7	10.4	56	17	715.4	205.3	0.278	181.298	94	94
32	2532.9	2551.3	27.2	1932	446	729.9	211.2	19.435	-189.313	-249.223	-249.223
33	2560	2565.1	12.3	315	75	729.9	211.2	1.906	-206.962	-265.568	-265.568
34	2572.4	2577.8	11.5	176	42	729.9	211.2	1.345	-187.236</		

1222 CONT

37	2616.5	2621.7	15.3	64	17	701.8	202.6	-0.243	-505.635	-542.189	-542.189
38	2660.6	2667.5	15.7	580	144	551.1	188.2	3.57	-139.888	-203.45	-203.45
39	2676.2	2682.5	12.7	229	56	551.1	188.2	1.603	-175.33	-236.273	-236.273
40	2689	2696.1	17.1	210	51	551.1	188.2	2.016	-190.163	-250.01	-250.01
41	2706.1	2709.5	9.2	73	17	551.1	188.2	0.424	-250.466	-305.857	-305.857
42	2722.2	2727.7	15.9	199	51	571.6	172	0.651	-100.806	-167.257	-167.257
43	2777.2	2797	30.7	236	60	452.9	143.2	2.109	-145.88	-209	-209
44	2807.9	2817.9	18	169	41	452.9	143.2	1.374	-179.803	-240.416	-240.416
45	2825.9	2834.5	18.8	156	37	452.9	143.2	1.658	-215.818	-273.789	-273.789
46	2871.7	2877.1	19.6	65	18	473.4	146.5	-0.166	-538.645	-572.739	-572.739
47	2953.8	2970.9	30.5	117	31	390.4	126.4	1.17	-133.727	-197.745	-197.745
48	2984.3	3000.2	27	193	48	390.4	126.4	2.136	-174.702	-235.691	-235.691
49	3011.3	3023.4	26.3	168	40	390.4	126.4	2.199	-200.635	-259.708	-259.708
50	3230.5	3251.2	35.7	167	43	323.8	108.3	2.948	-103.418	-169.676	-169.676
51	3266.3	3288	36.6	229	54	323.8	108.3	4.473	-165.135	-226.831	-226.831
52	3302.8	3319.5	33.6	68	17	323.8	108.3	1.596	-154.102	-216.614	-216.614
53	3484.2	3486.3	32.2	831	138	254.9	94.7	24.52	-445.053	-486.063	-486.063
54	3582.5	3586.2	35.7	829	138	253.2	94.2	24.578	-443.383	-484.517	-484.517

Triplicate 2

1	19.4	27	21.7	824	137	254.9	94.9	16.157	-447.206	-488.057	-488.057
2	99.1	100.3	21.7	822	137	254.2	94.5	16.123	-446.111	-487.044	-487.044
3	198.6	202.5	21.9	821	137	254.8	94.3	16.165	-444.621	-485.664	-485.664
4	297.8	302.4	22.2	820	137	253.1	94.4	16.086	-446.036	-486.974	-486.974
5*	869.6	884.3	44.3	3998	984	256.4	95.2	29.936	0	-73.9	-73.9
6	1610.1	1615.6	23	346	83	256	94.5	1.752	-187.395	-247.446	-247.446
7	1698.3	1704.4	15.3	70	18	262.1	95.2	0.344	-110.977	-176.676	-176.676
8	1784.2	1792	19.6	637	145	259.5	94.9	3.017	-193.277	-252.894	-252.894
9	1867.8	1873.3	16.3	103	26	267.7	96.3	0.483	-124.154	-186.879	-186.879
10	1946	1956.9	27.4	1081	233	265.8	96.1	5.618	-200.273	-259.373	-259.373
11	2026	2031.7	14.4	145	34	279.2	99.5	0.642	-215.948	-273.89	-273.89
12	2100.7	2109.4	21.9	513	120	273.6	97.4	2.417	-176.807	-237.641	-237.641
13	2174.6	2182.6	18.8	103	26	275.7	97.9	0.51	-147.272	-210.289	-210.289
14	2247.2	2255.3	20.5	187	46	275.8	97.9	0.924	-166.246	-227.86	-227.86
15	2336.2	2341.4	12.5	62	16	282.1	98.5	0.293	-84.059	-151.747	-151.747
16	2388.5	2394.1	11.7	51	12	284.9	100.1	0.255	-161.525	-223.488	-223.488
17	2558.8	2598.5	62.1	125	28	304.3	104.3	3.808	-191.544	-251.289	-251.289
18	3097	3135	63.1	107	25	301.8	104	3.646	-218.464	-276.22	-276.22
19	3483.4	3487.2	32.2	787	131	252.1	94.1	23.238	-447.198	-488.05	-488.05
20	3582.3	3585.4	33.2	783	130	251.7	94.1	23.231	-446.86	-487.737	-487.737

Triplicate 3

1	19.4	30.3	22.8	775	129	255	94.7	15.19	-455.192	-495.454	-495.454
2	99.1	105.1	21.9	774	129	253.1	93.8	15.167	-452.198	-492.68	-492.68
3	198.8	204.6	22.8	773	129	253.3	94	15.224	-452.035	-492.529	-492.529
4	297.8	307.4	22.2	771	129	253.9	93.5	15.107	-450.362	-490.98	-490.98
5*	932.1	940.1	24.2	1552	391	255.1	94.5	7.067	0	-73.9	-73.9
6	1276.2	1280.8	14.6	95	25	260	95.5	0.409	-96.288	-163.072	-163.072
7	1381.9	1386.1	17.8	100	26	263.6	96.3	0.424	-134.419	-198.386	-198.386
8	1406.6	1412.2	14.8	135	31	263	96.1	0.558	-227.631	-284.709	-284.709
9	1480.6	1487	14.6	222	56	259.8	95.2	0.894	-139.534	-203.122	-203.122
10	1575.4	1584.2	17.6	274	68	260.4	95.4	1.137	-157.608	-219.861	-219.861
11	1671	1679.5	20.1	1009	216	263.5	95.9	4.491	-197.295	-256.614	-256.614
12	1759.8	1766.9	17.3	394	95	265.9	96.4	1.658	-173.414	-234.498	-234.498
13	1846.3	1855.3	21.3	1050	230	264.3	95.5	5.125	-198.349	-257.591	-257.591
14	1929.5	1936.2	17.1	455	108	269.8	97.2	1.968	-185.802	-245.971	-245.971
15	2007.4	2018.9	27.4	1153	247	270.2	96.3	5.78	-191.643	-251.381	-251.381
16	2087.5	2095	20.3	533	125	275.8	98.2	2.479	-185.954	-246.112	-246.112
17	2155.8	2174.2	31.8	1359	295	273.7	96.9	7.327	-189.624	-249.696	-249.696
18	2187.6	2194.1	16.3	209	48	273.7	96.9	1.134	-233.58	-290.218	-290.218
19	2238.8	2245.9	15.9	494	114	278.2	97.8	2.242	-173.586	-234.658	-234.658
20	2310.9	2319.7	19	903	204	281	98.7	4.367	-184.525	-244.789	-244.789
21	2345.8	2352.3	19.4	150	34	284.9	99.7	0.732	-252.984	-308.188	-308.188
22	2380.9	2387.6	13	194	48	279.6	98	0.896	-148.956	-211.848	-211.848
23	2398.3	2404.3	15.7	275	61	292.1	101	1.206	-233.742	-290.388	-290.388
24	2421.3	2427.3	15.5	62	15	285.7	99.3	0.374	-204.439	-263.231	-263.231
25	2448.4	2456.4	19	311	76	283.6	98.9	1.446	-163.23	-225.067	-225.067
26	2505.9	2511.6	12.3	182	43	289.2	100.3	0.841	-211.908	-270.148	-270.148
27	2580.7	2587	12.1	52	13	288.2	100.7	0.245	-242.89	-298.841	-298.841
28	3483.6	3492.2	31.8	740	123	254.5	94.5	21.847	-455.946	-496.152	-496.152
29	3583.1	3587.7	31.8	737	123	253.9	94.1	21.825	-453.987	-494.337	-494.337

Triplicate 4

1	19.2	29.5	21.9	726	121	255.2	94.5	14.24	-446.641	-487.534	-487.534
2	99.1	114.3	21.7	724	120	255.6	94.6	14.177	-447.199	-488.051	-488.051
3	198.6	216.3	21.7	723	120	254.8	94.3	14.256	-446.822	-487.516	-487.516
4	298	303.7	22.6	721	120	255.8	94.2	14.129	-443.767	-484.873	-484.873
5	833.1	837.7	12.7	51	15	254.2	94	0.292	-20.065	-92.482	-92.482
6*	867.1	893.1	47.4	8468	2301	254.5	93.9	101.197	0	-73.9	-73.9
7	1213	1217	17.3	89	24	260.4	95.3	0.388	-117.604	-182.813	-182.813
8	1317.7	1321.9	14.6	94	25	262.1	95.4	0.389	-84.664	-152.308	-152.308
9	1343.2	1347.6	14.8	124	27	259.9	95.2	0.509	-234.246	-290.835	-290.835
10	1416	1422.9	19.2	218	55	259.3	94.4	0.9	-132.343	-196.463	-196.463
11	1514	1519.8	15.3	270	67	258.1	94.9	1.093	-142.242	-205.63	-205.63
12	1606.8	1614.9	20.7	960	207	261	94.9	4.357	-187.086	-247.16	-247.16
13	1695.6	1702.5	18.8	389	94	263.1	94.5	1.631	-123.279	-188.069	-188.069
14	1779.8	1790.5	25.3	1057	223	262.6	95.3	4.986	-195.877	-255.302	-255.302
15	1865.1	1871.6	19.2	444	106	267.3	95.2	1.625	-129.871	-194.173	-194.173
16	1945.2	1954.2	21.9	1120	240	266.2	95.8	5.607	-189.238	-249.153	-249.153
17	2023.1	2030.2	19.6	536	126	273	97	2.514	-171.625	-232.842	-232.842
18	2099.6	2109.6	22.6	1371	291	273.1	97.6	7.35	-193.562	-253.158	-253.158
19	2122.6	2128.5	16.5	194	44	288.9	100	0.867	-211.728	-269.981	-269.981
20	2172.6	2181.1	18.4	493	116	276.1	97.2	2.39	-173.021	-234.135	-234.135
21	2245.5	2254.9	20.9	901	204	274.7	96.9	4.552	-179.921	-240.524	-240.524
22	2278.5	2286.9	21.7	139	31	282.6	98.6	0.737	-211.341	-269.623	-269.623
23	2316.1	2322.8	16.5	197	48	275.5	96.9	0.97	-168.237	-229.704	-229.704
24	2332.6	2338.9	17.3	279	62	275.5	96.9	1.388	-182.235	-287.121	-287.121
25	2355.8	2361.7	15.5	57	14	285.5	98.9	0.321	-184.617	-244.874	-244.874
26	2385.1	2391.6	17.1	307	75	280	97.6	1.408	-140.794	-204.29	-204.29
27	2440.3	2445.9	13.2	173	39	284.5	99.3	0.814	-222.563	-280.016	-280.016
28	2517	2522.2	11.7	55	14	281.7	98.8	0.269	-188.112	-248.111	-248.111
29	3483.2	3487.6	32	692	115	253.6	93.7	20.428	-446.11	-487.043	-487.043
30	3582.9	3591.7	33.2	690	115	252.9	94	20.454	-447.016	-487.883	-487.883

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Triplicate 5																			
1	19.4	26.3	21.7	682	113	255.8	94.4	13.332	-448.065	-488.853	-488.853								
2	99.1	102.8	21.7	681	113	253.6	94	13.333	-448.101	-488.886	-488.886								
3	198.6	212.1	21.9	679	113	254.1	94.1	13.379	-448.464	-489.222	-489.222								
4	297.8	301.8	22.6	679	112	253.2	94.4	13.321	-451.304	-491.852	-491.852								
5	365.3	379.5	36.6	658	193	253	93.7	16.487	-9.003	-82.238	-82.238								
6	401.9	402.7	16.1	113	33	253	93.7	0.835	52.561	-25.223	-25.223								
7	418	424.3	12.3	1279	351	253	93.7	3.705	-13.499	-86.401	-86.401								
8	430.3	433	17.3	123	34	253	93.7	0.912	-49.529	-119.789	-119.789								
9*	1004	1015.1	34.1	2137	518	256.2	94.9	10.874	0	-73.9	-73.9								
10	1349.5	1354.1	13	151	40	265	96.3	0.596	-89.445	-156.735	-156.735								
11	1454.6	1459.2	12.7	156	41	266.7	96.5	0.83	-89.392	-156.686	-156.686								
12	1479.9	1484.7	14.8	218	48	266.5	97	0.849	-250.718	-306.09	-306.09								
13	1555	1560.6	17.3	335	83	264.9	95.7	1.371	-124.439	-189.143	-189.143								
14	1650.9	1657.8	18.4	412	100	265.1	96.4	1.707	-154.536	-217.016	-217.016								
15	1743.3	1753.7	29.1	1318	271	265	96	6.496	-194.644	-254.159	-254.159								
16	1832.1	1840.7	21.5	567	132	267.9	96.7	2.459	-169.973	-231.312	-231.312								
17	1919	1929.3	26.3	1362	284	267.7	96.3	6.914	-195.121	-254.601	-254.601								
18	2002.6	2010	21.3	654	150	271.4	97.4	2.863	-175.426	-236.362	-236.362								
19	2082.1	2092.5	21.1	1366	286	271.1	96.1	7.014	-161.055	-241.575	-241.575								
20	2159.8	2168.6	23.4	755	171	275.6	98	3.569	-178.686	-239.381	-239.381								
21	2237.3	2248.2	22.2	1748	365	279.4	98.5	9.989	-188.724	-248.677	-248.677								
22	2259.5	2265.8	18	296	66	279.4	98.5	1.524	-244.606	-300.429	-300.429								
23	2311.1	2318.9	15.9	689	156	280.3	99	3.2	-185.447	-245.642	-245.642								
24	2361.7	2372.1	20.1	62	15	284.3	99.6	0.289	-198.285	-257.531	-257.531								
25	2382.8	2393.3	20.3	1208	265	280.5	98.5	6.354	-183.971	-244.276	-244.276								
26	2414.8	2424	17.3	204	46	288.4	100	1.007	-217.828	-275.63	-275.63								
27	2454.1	2460.3	15.5	282	68	280.5	98.7	1.386	-196.773	-256.131	-256.131								
28	2469.5	2476	17.1	378	83	280.5	98.7	1.898	-251.045	-306.393	-306.393								
29	2492.7	2498.6	14.8	89	22	287.2	99.1	0.53	-155.78	-218.188	-218.188								
30	2521.2	2529.1	19	443	107	282.9	99	2.108	-169.2	-230.596	-230.596								
31	2570.7	2583	19.6	261	60	287.3	99.5	1.304	-192.642	-252.306	-252.306								
32	2590.3	2594.5	11.9	56	14	287.3	99.5	0.265	-183.964	-244.269	-244.269								
33	2654.1	2659.5	12.1	73	19	287.4	99.3	0.344	-62.695	-131.981	-131.981								
34	3483.4	3489.9	31.8	654	108	252.6	93.9	19.276	-449.538	-490.217	-490.217								
35	3583.1	3586.9	32.2	651	108	253.3	93.1	19.284	-444.176	-485.251	-485.251								
	T1	T2	T3	T4		T5, not used	Average	Stdev		T1		T3							
C23	-273.129		-256.614			-254.159	-255.3865	1.735947148		C16		892.8		940.1					
C25	-268.002		-257.591		-255.302	-254.601	-255.8313333	1.563704043		C23		1655.3		1679.5					
C27	-262.575		-251.381		-249.153	-241.575	-247.3696667	5.140488044		C25		1835		1855.3					
C29	-266.773	-259.373	-249.696		-253.158	-248.667	-252.7235	4.831341739		C27		2002.4		2018.9					
										C29		2171.7		2174.2					
							-252.82775			C36		2827		2827					

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Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs. VSMOW
Duplicate 1											
1	19.4	20.5	21.9	1240	203	33.3	25.2	23.714	-437.163	-478.757	-478.757
2	99.1	100.1	21.9	1233	202	33.3	25.2	23.627	-437.1	-478.698	-478.698
3	198.6	199.6	22.2	1235	201	33.3	25.3	23.657	-437.447	-479.02	-479.02
4	298	299.1	22.2	1239	200	33.4	25.5	23.396	-438.34	-479.847	-479.847
5	507.7	526.5	94	1762	494	37.2	26.2	37.657	-21.369	-93.69	-93.69
6	963.5	982.9	37.4	64	14	90	39.2	1.253	-289.48	-341.987	-341.987
7	1002.6	1017.6	72.5	301	65	107.2	42.2	6.858	-220.282	-277.903	-277.903
8*	1141.8	1180.8	126.4	4627	1366	68.9	34.6	131.55	0	-73.9	-73.9
9	1281.4	1300.2	66	127	30	74.2	35.8	3.896	-144.325	-207.559	-207.559
10	1429.6	1450.5	78.6	108	27	122.2	48.4	1.954	-114.956	-180.361	-180.361
11	1564.2	1610.8	72.7	392	90	101.2	41.7	11.814	-207.298	-265.879	-265.879
12	1680.8	1705.6	54.3	76	15	145.4	50.6	1.737	-287.561	-340.21	-340.21
13	1736.2	1776.1	78	252	56	134.7	48.8	10.139	-250.145	-305.56	-305.56
14	1815.2	1848.4	62.1	574	114	242.3	71	12.981	-290.868	-343.271	-343.271
15	1912.9	1939.5	68.1	398	91	119.8	46	11.048	-191.752	-251.481	-251.481
16	2055.1	2103.2	76.7	355	82	112.5	44.1	10.819	-197.017	-256.358	-256.358
17	2232.7	2278.5	124.4	1622	359	85.9	37.9	53.429	-210.222	-268.587	-268.587 C23
18	2360.7	2427.5	134.4	791	178	122.9	46.7	25.535	-201.026	-260.07	-260.07
19	2545.2	2592.9	116.2	1818	404	70.5	34.3	60.296	-207.728	-266.276	-266.276 C25
20	2697.1	2732.3	82.8	855	194	90.7	38.7	25.301	-190.894	-250.687	-250.687
21	2839.5	2895.5	144.6	2279	519	89.8	38.1	87.91	-198.391	-257.629	-257.629 C27
22	2984.7	3024.4	96.6	1114	255	132.3	47.7	36.763	-191.795	-251.521	-251.521
23	3116.4	3200.8	124.1	3989	945	109	42.2	200.845	-197.093	-256.427	-256.427 C29
24	3240.5	3244.3	25.1	493	113	109	42.2	8.036	-214.291	-272.355	-272.355
25	3265.6	3302.4	103.5	1634	364	109	42.2	50.132	-196.133	-255.538	-255.538
26	3371	3455.6	130	3389	798	133.4	45.4	155.264	-191.697	-251.43	-251.43
27	3501.4	3516.8	27.6	151	26	378.2	105.9	1.607	-438.403	-479.905	-479.905
28	3529	3551.1	42	528	113	378.2	105.9	7.993	-226.942	-284.071	-284.071
29	3571	3596.7	47.7	588	113	378.2	105.9	10.246	-339.72	-388.515	-388.515
30	3618.6	3626.8	16.1	53	4	378.2	105.9	0.221	-1670.184	-1620.657	-1620.657
31	3634.7	3669.8	95.5	1376	313	378.2	105.9	29.132	-207.907	-266.443	-266.443
32	3744.7	3769.3	84	536	119	149.1	51.5	12.918	-233.525	-290.168	-290.168
33	3841.8	3877.8	76.9	307	70	89.9	37.6	8.184	-177.497	-238.28	-238.28
34*	3956.6	4025.8	128.1	2451	563	101.8	40.7	99.744	0	-244.1	-244.1
35	4085.3	4097.7	29.1	81	14	105.8	42.5	0.808	-33.164	-269.168	-269.168
36	4996.1	4997.2	101.6	982	157	43.2	28.3	93.675	-307.712	-476.7	-476.7
37	5115.7	5116.5	61.9	992	158	33.5	25	56.507	-301.287	-471.843	-471.843
Duplicate 2											
1	19.4	20.5	21.9	958	155	33.4	25.2	18.328	-439.934	-481.323	-481.323
2	99.1	100.1	21.9	953	154	33.4	24.9	18.258	-439.345	-480.777	-480.777
3	198.6	199.6	22.2	956	154	33.5	25.1	18.274	-440.057	-481.437	-481.437
4	298	299.1	21.9	959	153	33.5	25.1	18.087	-440.801	-482.126	-482.126
5	506.2	522.5	103.5	690	192	42	27.3	22.832	-16.635	-89.306	-89.306
6	1001.9	1016.4	70	227	48	87.9	38.2	4.902	-290.635	-290.635	-290.635
7*	1142.4	1169.4	116.4	2278	648	55.7	31.4	53.355	0	-73.9	-73.9
8	1281.2	1296.6	29.1	90	22	61.1	32.2	1.508	-146.76	-209.815	-209.815
9	1432.1	1447.3	67.9	79	19	91.4	39.2	1.419	-155.621	-218.021	-218.021
10	1589	1606	45.4	288	66	110	42.4	5.567	-170.556	-231.852	-231.852
11	1678.3	1701.5	48.7	66	14	105.5	41.5	1.244	-269.876	-323.832	-323.832
12	1738.3	1770.4	48.1	209	46	99	40.6	4.498	-241.033	-297.12	-297.12
13	1809.7	1843.6	64.4	478	96	149.1	50.7	9.533	-285.924	-338.694	-338.694
14	1912.1	1934.1	67.3	318	71	87.6	38.1	7.082	-186.199	-246.339	-246.339
15	2080	2097.7	50.8	283	64	103.1	41.2	5.456	-171.837	-233.038	-233.038
16	2228.1	2272.7	88	1202	262	67.7	33.3	31.639	-209.339	-267.769	-267.769 C23
17	2374.7	2422.3	119.5	593	131	98.3	40.5	14.969	-196.88	-256.23	-256.23
18	2548.3	2586.8	103	1328	291	57	30.8	37.74	-204.984	-263.736	-263.736 C25
19	2699.9	2727	76.9	691	153	67.5	33	16.034	-188.129	-248.126	-248.126
20	2842.8	2888	111.8	1689	377	66.1	33	54.691	-200.909	-259.962	-259.962 C27
21	2987.4	3018.8	89.2	933	206	88.2	37.6	23.62	-193.236	-252.856	-252.856
22	3121.2	3188.9	142.5	2981	686	80.1	35.8	129.445	-197.761	-257.047	-257.047 C29
23	3264.2	3297.6	91.8	1073	237	113.1	43.6	27.335	-201.603	-260.605	-260.605
24	3382.2	3449.5	109.1	2452	563	95.8	39	93.741	-191.112	-250.888	-250.888
25	3492	3507.6	37.4	66	11	272.6	81.3	-0.492	534.333	420.946	420.946
26	3529.4	3548.6	39.9	375	80	272.6	81.3	3.63	-250.257	-305.663	-305.663
27	3569.3	3592.1	47	381	71	272.6	81.3	5.354	-377.602	-423.597	-423.597
28	3639.7	3670.2	91.3	1051	236	174.1	58.2	24.703	-180.253	-240.832	-240.832
29	3751.1	3778.8	74.4	365	77	104.7	40.9	7.935	-221.668	-279.187	-279.187
30	3845.8	3876.7	70.9	216	49	72.4	33.6	5.049	-166.575	-228.165	-228.165
31*	3964.9	4002.6	100.9	1100	246	80	35.9	29.101	0	-244.1	-244.1
32	4258	4300.8	86.5	59	14	72.2	34.2	2.62	19.707	-229.203	-229.203
33	4995.9	4997	101.6	767	121	43.6	28.4	72.584	-316.11	-483.047	-483.047
34	5115.5	5116.3	61.9	788	122	33.4	25.2	43.911	-308.539	-477.325	-477.325

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Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vss)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs. VSMOW
Duplicate 1											
1	19 4	20 3	21 7	710	111	28 5	22 2	13 388	-450 729	-491 32	-491 32
2	99 1	99 9	21 7	717	111	28 5	22 2	13 373	-450 289	-490 913	-490 913
3	198 6	199 4	21 9	706	112	28 5	22	13 441	-448 75	-489 487	-489 487
4	298	299 1	21 7	705	111	28 5	22 2	13 336	-449 73	-490 395	-490 395
5	442 7	456	81 7	1223	336	29 8	22 1	21 829	-23 154	-95 343	-95 343
6*	1075 5	1090 6	92	1659	461	35 6	24	32 534	0	-73 9	-73 9
7	1312 9	1320	38	57	14	40 9	25 2	9 904	-187 487	-247 532	-247 532
8	1422 5	1430 6	38 5	115	26	44 8	25 6	1 839	-175 825	-236 546	-236 546
9	1523 4	1535 1	45 4	104	24	49 9	26 9	1 867	-202 845	-281 754	-281 754
10	1576 5	1588 1	28 2	88	15	54 1	27 5	0 887	-235 864	-292 334	-292 334
11	1628 5	1636 9	42 6	192	43	53 9	27 7	2 687	-176 532	-237 386	-237 386
12	1723 4	1733 9	55 2	232	52	42 8	25 4	3 691	-186 001	-246 155	-246 155
13	1815 2	1831 9	76 5	820	178	42 9	25	14 547	-198 935	-258 134	-258 134
14	1905 5	1917 2	56 6	358	78	46 9	26 4	5 624	-196 928	-256 275	-256 275
15	1989 9	2006 8	57 7	794	172	43 8	25 3	13 699	-203 707	-262 553	-262 553
16	2074 1	2086 2	38 5	409	90	49 5	26 8	6 146	-196 487	-255 867	-255 867
17	2152 7	2170 9	55 2	965	216	49 6	26 3	17 401	-194 804	-254 308	-254 308
18	2232 1	2249 8	70 9	804	134	74	32 2	9 334	-184 867	-245 105	-245 105
19	2304 4	2331 6	60 4	1923	424	58 1	26	37 901	-204 266	-263 071	-263 071
20	2364 8	2393 1	64 6	821	182	58 1	28 4	24 506	-217 718	-275 529	-275 529
21	2429 4	2435 3	19 4	87	20	56 1	28 4	1 222	-209 004	-267 458	-267 458
22	2448 9	2471	66	1433	319	58 1	28 4	29 998	-203 24	-262 12	-262 12
23	2514 9	2529 9	42 6	783	165	58 1	28 4	13 388	-233 108	-289 781	-289 781
24	2557 5	2601	88 2	1412	314	58 1	28 4	39 565	-218 28	-276 049	-276 049
25	2646 1	2656 2	21 1	177	40	114 9	42 1	1 882	-209 756	-268 155	-268 155
26	2667 3	2680 6	40 3	463	96	114 9	42 1	7 409	-259 979	-314 666	-314 666
27	2707 6	2724 3	63 5	944	216	114 9	42 1	16 882	-169 596	-230 963	-230 963
28*	2771 1	2806 2	81 3	2254	509	114 9	42 1	54 429	0	-244 1	-244 1
29	2852 4	2859 5	37 4	70	17	114 9	42 1	-0 072	-879 507	-908 919	-908 919
30	3483	3483 8	31 6	689	106	28 9	22 1	19 211	-310 979	-479 169	-479 169
31	3582 5	3583 3	31 8	688	106	28 5	21 6	19 261	-309 098	-477 747	-477 747
Duplicate 2											
1	19 4	20 5	21 7	671	105	28 5	22 3	12 689	-451 508	-492 041	-492 041
2	99 1	99 9	21 7	667	105	28 5	22 3	12 678	-451 481	-492 016	-492 016
3	198 6	199 6	21 9	670	105	28 5	22 1	12 729	-450 222	-490 851	-490 851
4	298	299 1	21 7	672	105	28 5	22 1	12 642	-450 342	-490 962	-490 962
5	442	456	82 3	1407	386	30	22 4	25 247	-27 044	-98 945	-98 945
6*	1076 1	1097 5	96 8	1822	507	35 9	24	36 187	0	-73 9	-73 9
7	1313 1	1320	38	58	14	41 1	24 9	0 93	-115 71	-181 059	-181 059
8	1422 5	1430 8	39 2	117	27	45	25 6	1 884	-187 551	-229 069	-229 069
9	1523 8	1535 1	44 9	106	25	50 3	26 6	1 693	-197 453	-228 978	-228 978
10	1576 7	1586 1	28 2	70	15	54 5	27 7	0 889	-244 148	-300 006	-300 006
11	1628 9	1637 1	42 2	196	44	53 7	27 7	2 748	-172 68	-233 819	-233 819
12	1724 7	1734 1	53 9	238	54	42 9	25 1	3 782	-165 943	-227 58	-227 58
13	1817 3	1832 1	74 8	838	181	42 9	25 3	14 635	-205 516	-264 228	-264 228
14	1906 7	1917 4	55 6	367	81	46 8	26 4	5 782	-196 829	-256 183	-256 183
15	1992	2007	56	816	176	44	25 7	14 018	-207 178	-265 788	-265 788
16	2075 4	2086 4	37 4	420	93	49 2	26 8	6 306	-192 897	-252 542	-252 542
17	2154 6	2171 3	53 5	1014	222	49 2	26 6	17 873	-198 324	-257 568	-257 568
18	2234 2	2247 2	74 2	626	137	69 4	31 4	9 886	-189 683	-249 565	-249 565
19	2310 5	2332 2	54 5	1976	435	55 9	27 9	38 784	-204 742	-263 512	-263 512
20	2365	2393 5	64 6	845	187	55 9	27 9	25 37	-217 569	-275 391	-275 391
21	2429 5	2435 7	23 6	93	21	55 9	27 9	1 453	-203 406	-262 274	-262 274
22	2453 2	2471 6	62 7	1479	329	55 9	27 9	30 897	-202 26	-261 213	-261 213
23	2515 9	2530 4	41 8	805	170	55 9	27 9	13 76	-232 241	-288 979	-288 979
24	2557 7	2601 4	88 2	1454	324	55 9	27 9	40 88	-217 713	-275 524	-275 524
25	2646 6	2656 4	21 3	188	42	118 5	42 9	2 03	-201 169	-260 203	-260 203
26	2667 9	2681 1	40 8	478	98	118 5	42 9	7 653	-255 851	-310 843	-310 843
27	2708 6	2724 7	65	977	223	118 5	42 9	17 446	-168 572	-230 015	-230 015
28*	2773 6	2808 3	79 8	2457	557	118 5	42 9	60 542	0	-244 1	-244 1
29	2853 5	2860 4	37	78	19	118 5	42 9	0 023	4280 096	2991 225	2991 225
30	3483	3483 8	31 8	650	101	28 9	22 1	18 21	-310 381	-478 717	-478 717
31	3582 5	3583 3	31 8	639	101	28 5	21 9	18 269	-308 081	-476 978	-476 978
Duplicate 3											
1	19 4	20 3	22 6	2554	424	33 2	25 3	47 965	-431 62	-473 623	-473 623
2	99 1	99 9	22 6	2550	423	33 2	25 6	47 82	-432 255	-474 211	-474 211
3	198 6	199 4	22 8	2541	422	33 2	25 5	48 041	-432 058	-474 029	-474 029
4	298	298 9	22 8	2503	421	33 3	25 4	47 675	-431 795	-473 785	-473 785
5	508 7	528 6	99 1	2075	584	37	26 7	45 431	-22 53	-94 765	-94 765
6	638	1032 7	145 9	138	32	51 2	29 8	9 484	-204 384	-263 16	-263 16
7*	1142 2	1185 2	136 9	5276	1565	84	38 9	161 518	0	-73 9	-73 9
8	1282 2	1308 1	94 7	304	69	82 2	38 2	11 391	-180 276	-240 853	-240 853
9	1388 2	1457 4	130	314	72	99 8	42 4	13 447	-216 35	-274 262	-274 262
10	1520 1	1551 2	63 7	59	12	137 5	49 9	2 13	-324 374	-374 303	-374 303
11	1584 4	1621 2	105 1	556	128	143 7	50 4	25 53	-194 588	-254 108	-254 108
12	1737 6	1782 8	81 7	421	97	219 4	96	16 122	-163 743	-244 065	-244 065
13	1819 3	1852 6	94 5	256	53	219 4	96	11 839	-212 776	-270 954	-270 954
14	1913 8	1952 3	118 9	751	176	219 4	96	26 598	-121 887	-186 78	-186 78
15	2073 3	2119 3	158 8	672	201	112 8	45 4	44 318	-186 42	-246 544	-246 544
16	2233 4	2309	164 5	3510	811	105 9	44	172 174	-202 539	-261 472	-261 472
17	2398 7	2446 5	148 2	1446	335	125 9	46 8	67 12	-235 376	-235 376	-235 376
18	2548 3	2624 4	154 7	3277	756	106 3	43 5	165 715	-194 835	-254 336	-254 336
19	2703 4	2758 2	140 9	1472	343	148 2	53 8	80 624	-184 461	-244 729	-244 729
20	2844 9	2932 3	151 5	3432	812	156 2	54 1	212 752	-184 397	-244 67	-244 67
21	2996 4	3059 3	134 2	1882	401	156 2	54 1	123 98	-170 589	-231 883	-231 883
22	3130 6	3261 9	162 4	6554	1611	156 2	54 1	502 084	-191 495	-251 243	-251 243
23	3293	3323 9	116	3902	865	156 2	54 1	223 486	-200 434	-259 522	-259 522
24	3409	3506	133 6	5031	1218	156 2	54 1	331 982	-188 326	-246 456	-246 456
25	3542 6	3711	180 2	4963	1226	156 2	54 1	444 865	-212 872	-271 041	-271 041
26	3725 2	3732 3	54 5	95	8	4867 3	1226 6	-150 576	-282 606	-100 392	-100 392
27	3841	3852 5	43 9	175	20	2727 1	635 1	-45 421	-127 44	-191 822	-191 822
28	3884 9	3947	107 2	1341	376	2727 1	635 1	-89 504	-295 075	-347 169	-347 169
29*	3992 1	4048 3	102 2	672	181	2727 1	635 1	-136 942	0	-244 1	-244 1
30	4304 6	4324 6	35 7	52	13	121 3	44 9	0 993	251 974	-53 633	-53 633
31	4619 9	4678 7	89 5	69	16	101 9	41 5	3 785	32 061	-219 865	-219 865
32	4996 8	4997 6	102 4	2298	376	53	31	215 61	-269 612	-447 9	-447 9
33	5116 1	5117 2	62 9	2262	377	33 7	26 1	130 177	-267 085	-445 99	-445 99
Duplicate 4											
1	19 4	20 5	22 6	2231	373	33 4	26	42 586	-432 807	-474 723	-474 723
2	99 1	100 1	22 6	2237	373	33 5	25 7	42 428	-432 428	-474 372	-474 372
3	198 6	199 6	22 8	2239	372	33 5	25 6	42 626	-432 123	-474 089	-474 089
4	298 2	298 1	22 6	2250	371	33 5	26	42 289	-433 046	-474 944	-474 944
5	508 3										

1422 CONT

11	1584 2	1617 9	104 5	554	126	140 7	50	24 933	-197 24	-256 564	-256 564
12	1689 8	1714 8	46	56	12	186 4	60 2	1 64	-320 033	-370 283	-370 283
13	1737	1778 8	81 7	431	99	209 1	64 1	16 148	-189 711	-249 591	-249 591
14	1818 7	1848 4	57 3	267	55	209 1	64 1	9 513	-261 856	-316 405	-316 405
15	1913 8	1940 1	118 1	777	178	207 2	68	26 598	-200 988	-260 035	-260 035
16	2073 3	2115 7	158 8	901	208	110 3	45 2	42 978	-196 75	-256 11	-256 11
17	2233 4	2306 5	164 1	3628	831	103 3	43 4	166 625	-212 186	-270 405	-270 405
18	2396 3	2445 3	148 2	1513	347	122 1	46	64 62	-200 298	-259 364	-259 364
19	2547 9	2621 3	154 7	3393	776	104 8	43 2	159 59	-207 777	-266 323	-266 323
20	2703 4	2753 2	140 7	1540	359	144 1	52 5	78 112	-196 031	-255 445	-255 445
21	2844 9	2928 1	150 7	3581	844	153 7	53 2	204 913	-199 776	-258 913	-258 913
22	2998	3051 2	133 8	1578	375	294 9	66 5	100 163	-184 595	-244 853	-244 853
23	3130 2	3257 9	158 8	6358	1558	198 1	64 7	469 605	-210 661	-268 993	-268 993
24	3289	3319 1	118 1	3676	851	198 1	64 7	211 738	-222 861	-280 292	-280 292
25	3407 1	3501 2	129 8	4700	1133	198 1	64 7	302 299	-208 013	-266 541	-266 541
26	3536 9	3586	84 2	2709	601	198 1	64 7	144 736	-240 13	-296 285	-296 285
27	3621 1	3706 4	155 1	4747	1159	198 1	64 7	372 599	-225 677	-282 9	-282 9
28	3776 8	3846 5	106 4	2420	525	401 9	112 6	102 907	-245 917	-301 644	-301 644
29	3883 2	3940 5	105 3	3286	799	401 9	112 6	135 296	-165 537	-227 204	-227 204
30*	3988 6	4048 2	104 3	2991	899	401 9	112 6	100 793	0	-244 1	-244 1
31	4092 8	4112 5	58 7	343	76	401 9	112 6	-0 461	-584 839	-686 18	-686 18
32	4287	4352 8	177 9	118	27	152 4	53 3	7 17	-23 538	-261 862	-261 862
33	4996 8	4997 8	102 2	1990	330	55 8	32 4	190 336	-301 901	-472 307	-472 307
34	5116 3	5117 2	62 7	2013	331	33 8	26 4	115 249	-297 661	-469 117	-469 117

Duplicate 5 (F)

1	19 4	20 5	22 2	1046	167	51	20 3	19 919	-445 498	-502 778	-502 778
2	99 1	100 1	22 2	1044	166	51 1	21	19 889	-447 761	-504 807	-504 807
3	198 6	199 6	22 4	1049	166	51 1	20 8	19 977	-446 7	-503 856	-503 856
4	298 2	299 1	21 9	1051	166	51 2	21	19 814	-447 524	-504 595	-504 595
5	1134 7	1148 7	52	128	32	63 2	24	2 689	-75 202	-170 734	-170 734
6	1269 3	1287 6	64 4	137	32	66 5	24	3 863	-158 786	-245 683	-245 683
7	1416	1436 5	70 4	145	34	81 4	28	3 951	-169 328	-255 136	-255 136
8	1567 3	1595 3	64 8	289	65	88 5	29 5	8 206	-190 901	-274 481	-274 481
9	1718 6	1757 5	78 8	233	53	106 1	33 1	6 862	-198 035	-280 878	-280 878
10	1798 9	1825 2	56	157	32	107 6	33 8	4 214	-290 358	-363 664	-363 664
11	1897 5	1924 5	81 7	437	98	96 6	32 4	12 12	-192 606	-276 01	-276 01
12	2058 4	2089 8	105 8	498	113	79 5	28	16 026	-190 252	-273 899	-273 899
13	2218 3	2266 6	119 5	1888	416	77 4	27 3	61 7	-213 43	-294 683	-294 683
14	2378 4	2413 1	99 5	794	178	82 2	28 3	24 478	-196 211	-278 243	-278 243
15	2529 7	2578 4	117 5	1794	396	76 5	26 8	59 423	-209 772	-291 402	-291 402
16	2680 6	2718 3	94 1	841	192	89 9	29 8	28 999	-191 884	-275 362	-275 362
17	2823 6	2879 6	143	2056	462	90 4	30 1	79 249	-207 768	-289 606	-289 606
18	2967 2	3013 2	127 1	1043	242	110 8	34 8	44 047	-193 67	-278 964	-278 964
19	3103 2	3190 4	118 5	3787	878	98 5	31 6	190 975	-222 013	-302 379	-302 379
20	3221 7	3240 1	38 4	1413	303	98 5	31 6	37 677	-249 08	-326 65	-326 65
21	3258 1	3288 4	98 8	1403	316	98 5	31 6	50 913	-202 723	-285 081	-285 081
22	3355 9	3439 9	116 4	2691	626	170 3	47 1	128 247	-209 907	-291 524	-291 524
23	3472 3	3511 2	58 7	1062	221	170 3	47 1	37 907	-247 223	-324 985	-324 985
24	3531 1	3596 5	83	1544	319	170 3	47 1	69 892	-249 77	-327 298	-327 298
25	3614	3673 6	113 7	2475	578	170 3	47 1	110 863	-200 429	-283 025	-283 025
26	3727 7	3780 8	106 4	1264	271	170 3	47 1	83 807	-233 246	-312 452	-312 452
27	3835 1	3896 4	119 8	2513	591	134 7	39 5	94 046	-175 747	-280 892	-280 892
28	3954 9	3996	33	141	33	134 7	39 5	1 896	-112 09	-203 811	-203 811
29	4050 2	4073	57 1	447	102	86 7	28 4	9 29	-153 643	-241 072	-241 072
30*	4375 8	4428 8	82 6	726	196	90 6	29 8	23 991	0	-103 3	-103 3
31	4996 1	4997 2	102	962	152	67 6	24 9	61 651	-451 509	-508 168	-508 168
32	5115 7	5116 5	62 1	975	154	51 2	20 7	55 784	-446 796	-503 942	-503 942
33	5115 5	5116 5	62 1	883	140	51 4	20 8	51 087	-435 684	-493 978	-493 978

Duplicate 6 (F)

1	19 4	20 3	21 9	963	153	51 2	20 4	18 253	-433 738	-492 233	-492 233
2	99 1	99 9	21 9	965	152	51 3	21	18 226	-436 069	-494 323	-494 323
3	198 6	199 4	22 2	950	151	51 3	21	18 31	-436 071	-494 325	-494 325
4	298	299 1	21 9	950	151	51 4	21 2	18 159	-437 178	-495 318	-495 318
5	1137	1151 4	50 4	108	28	61 8	23 4	2 322	-33 535	-133 371	-133 371
6	1272	1290 4	64 6	114	27	64 7	23 6	3 248	-95 357	-188 806	-188 806
7	1418 7	1439 4	69 6	119	28	77 3	27 1	3 304	-160 347	-247 083	-247 083
8	1570 8	1598 4	63 7	239	54	83 2	28 3	6 913	-178 749	-261 791	-261 791
9	1722	1760 6	78 6	196	45	98 6	31 3	5 771	-175 059	-260 275	-260 275
10	1801 6	1826 3	58 4	131	27	99 8	31 8	3 542	-259 327	-335 838	-335 838
11	1900 6	1927	77 1	368	83	92 2	31 2	10 189	-185 574	-269 705	-269 705
12	2061 6	2091 9	84 9	421	95	76 7	26 9	13 265	-181 346	-256 946	-256 946
13	2221 3	2266 6	117 9	1652	364	73 8	25 1	51 852	-182 353	-266 816	-266 816
14	2381 1	2414 2	96 1	677	152	77 8	28 3	20 62	-188 49	-272 319	-272 319
15	2532 2	2578 2	115 6	1568	344	73	26	50 166	-191 123	-274 68	-274 68
16	2682 9	2718 9	90 3	731	167	84 3	28 5	24 498	-173 541	-258 914	-258 914
17	2826 1	2878 3	142 1	1822	407	84 7	28 7	66 865	-188 683	-272 492	-272 492
18	2969 1	3012 5	117 2	944	218	101 1	32	37 305	-169 354	-255 16	-255 16
19	3105 3	3185 6	110 6	3392	779	92 1	30 1	158 308	-202 025	-284 456	-284 456
20	3216 5	3235 5	38 9	276	47	104 3	24 6	-3 42	89 419	-23 118	-23 118
21	3255 4	3285 7	97 4	279	60	104 3	24 6	-50 083	-187 188	-271 152	-271 152
22	3354 4	3435 5	113 1	2443	564	152 5	43	107 701	-190 962	-274 535	-274 535
23	3467 5	3508 8	59 1	921	192	152 5	43	32 059	-230 255	-309 769	-309 769
24	3526 7	3591 7	83 2	1365	281	152 5	43	59 315	-230 649	-310 123	-310 123
25	3609 8	3670 2	115	2211	511	152 5	43	94 059	-180 748	-265 377	-265 377
26	3725 2	3778 6	106 6	1083	230	169 9	48 2	35 067	-226 06	-307 801	-307 801
27	3833 5	3893 3	121 2	2226	521	122 8	37	79 112	-157 225	-244 283	-244 283
28	3955 1	3986 4	31 8	122	28	119 1	37 5	1 775	-208 658	-290 403	-290 403
29	4050 4	4074 7	60 8	365	84	84 9	28	8 036	-128 421	-218 455	-218 455
30	4153 9	4175 2	53 5	71	19	106 4	33 4	1 439	-17 968	-119 411	-119 411
31*	4377 9	4535 7	180 2	3215	908	92 8	29 9	277 043	0	-103 3	-103 3
32	4996 1	4997	101 6	898	140	70	28 1	83 645	-443 693	-501 16	-501 16
33	5115 5	5116 5	62 1	883	140	51 4	20 8	51 087	-435 684	-493 978	-493 978

152a

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Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs. VSMOW
Duplicate 1											
1	19.4	20.5	22.4	2506	422	33.5	26	47.766	-438.066	-479.593	-479.593
2	99.1	100.1	22.4	2502	421	33.6	26	47.705	-438.147	-479.668	-479.668
3	198.8	199.8	22.8	2519	421	33.6	26.2	47.889	-438.132	-479.654	-479.654
4	298.2	299.1	22.2	2529	420	33.7	26.2	47.539	-438.131	-479.653	-479.653
5	512.5	534.6	106	3557	1020	41.5	28.6	78.4	-30.122	-101.796	-101.796
6*	1139.5	1169.8	110.1	2409	692	45.1	29.1	58.257	0	-73.9	-73.9
7	1281.2	1295	53.5	79	19	46.9	29.7	1.651	-175.58	-236.504	-236.504
8	1428.9	1443.8	56.6	118	28	51.1	30.3	2.375	-153.517	-216.072	-216.072
9	1583.8	1603.9	59.1	250	57	55.2	30.9	4.911	-173.599	-234.671	-234.671
10	1735.3	1766.9	74.2	216	49	60.2	32.1	5.094	-199.79	-258.926	-258.926
11	1812.2	1838.8	59.6	271	54	62.5	32.8	5.466	-203.281	-345.508	-345.508
12	1912.1	1933.9	69.8	374	84	54.4	30.9	7.47	-186.82	-246.914	-246.914
13	2073.7	2099.2	73.4	430	96	47.6	29.2	9.168	-184.854	-245.093	-245.093
14	2232.7	2273.7	111	1208	266	48	29.3	33.333	-206.527	-265.165	-265.165
15	2392.4	2422.9	80.3	806	136	50.6	29.4	13.763	-181.681	-242.155	-242.155
16	2543.5	2586	108.1	1150	254	49	29.5	31.926	-203.714	-262.559	-262.559
17	2694.2	2727.9	83.6	659	147	53.5	30.5	15.938	-189.797	-249.671	-249.671
18	2837	2884.4	89.5	1366	305	56.3	30.9	40.363	-196.121	-255.528	-255.528
19	2980.3	3020.1	102.6	839	188	63.8	32.7	22.09	-186.656	-246.762	-246.762
20	3113.9	3179.1	91.5	1927	433	63.5	33	67.841	-201.263	-260.289	-260.289
21	3205.4	3227.6	52.3	753	161	63.5	33	24.17	-244.753	-300.566	-300.566
22	3258.1	3290.5	61.2	662	147	167.7	57.1	13.752	-194.934	-254.428	-254.428
23	3358.4	3438.1	115.4	1660	376	87.3	37.8	62.567	-200.444	-259.531	-259.531
24	3473.8	3507	56.2	540	113	87.3	37.8	16.9	-244.39	-300.229	-300.229
25	3530	3592.5	85.1	769	158	87.3	37.8	30.482	-238.269	-294.561	-294.561
26	3615.1	3674.2	116.8	1361	314	87.3	37.8	53.024	-189.156	-249.077	-249.077
27	3732.9	3782.9	104.1	669	144	108.6	42.9	19.661	-226.912	-284.043	-284.043
28	3841.6	3897.6	115.4	1244	292	76.4	35.6	39.202	-158.396	-220.591	-220.591
29*	3958.3	4021	117.7	1960	450	79.8	36.8	70.276	0	-244.1	-244.1
30	4077.2	4099.1	57.7	137	33	83.6	38.1	2.391	28.624	-222.463	-222.463
31	4995.9	4997	102.2	2311	387	42.9	28.4	221.598	-296.684	-468.364	-468.364
32	5115.5	5116.3	62.3	2337	367	33.8	25.7	133.257	-295.146	-467.201	-467.201
Duplicate 2											
1	19.4	20.3	22.2	2321	363	33.7	26.1	43.648	-436.891	-478.505	-478.505
2	99.1	99.9	22.2	2306	363	33.7	26.1	43.525	-436.72	-478.346	-478.346
3	198.6	199.4	22.4	2297	362	33.7	25.9	43.762	-436.644	-478.276	-478.276
4	298	299.1	22.4	2275	362	33.8	25.7	43.449	-436.189	-477.854	-477.854
5	512.7	534.6	104.7	3611	1035	42.3	28.4	78.432	-28.439	-100.238	-100.238
6*	1140.1	1170	108.5	2475	711	45.2	29.2	60.123	0	-73.9	-73.9
7	1281.2	1295	54.1	85	20	46.8	29.4	1.77	-181.838	-223.778	-223.778
8	1428.7	1443.8	57.5	125	30	51.8	30	2.52	-131.844	-196	-196
9	1584	1604.3	59.9	262	80	56.1	31.1	5.193	-182.619	-243.024	-243.024
10	1734.7	1767.1	75	227	52	61.4	32.4	5.418	-205.3	-264.029	-264.029
11	1813.1	1839.2	58.7	286	57	63.7	32.7	5.829	-282.693	-335.702	-335.702
12	1912.1	1934.3	69.4	393	88	54.7	30.8	7.87	-180.215	-240.797	-240.797
13	2074.3	2099.6	73.2	452	101	47.9	29.2	9.802	-180.627	-241.179	-241.179
14	2233.8	2274.8	110.1	1258	276	48.2	29.4	35.6	-206.172	-264.836	-264.836
15	2393.3	2423.8	80.3	634	142	51.1	29.8	14.733	-187.601	-247.638	-247.638
16	2544.8	2587	107.6	1194	264	49.5	29.5	34.217	-202.865	-261.773	-261.773
17	2695.1	2728.7	83.4	690	156	54.3	29.8	17.145	-173.634	-234.703	-234.703
18	2838.4	2885.9	89.2	1414	316	57.3	31.3	43.255	-197.323	-256.641	-256.641
19	2981.4	3021.5	103.5	864	194	65.1	32.9	23.767	-184.665	-244.918	-244.918
20	3116.2	3181.2	91.5	1980	445	64.8	33	73.448	-199.454	-256.614	-256.614
21	3207.7	3229.3	50.8	816	174	64.8	33	25.371	-240.873	-296.972	-296.972
22	3258.5	3292.2	62.5	792	178	64.8	33	21.833	-194.144	-253.697	-253.697
23	3390.3	3439.9	113.9	1701	386	91.9	38.7	67.116	-200.239	-259.341	-259.341
24	3474.6	3508.9	57.5	397	79	256	77.9	9.185	-311.542	-362.419	-362.419
25	3532.1	3547.4	34.9	287	63	256	77.9	4.7	-226.974	-283.175	-283.175
26	3567.6	3594.4	49.3	524	102	361.6	99.3	8.942	-302.058	-353.636	-353.636
27	3617	3676.3	116.8	1146	267	361.6	99.3	26.011	-140.077	-203.625	-203.625
28	3734.6	3784.8	104.5	697	151	114	44.3	21.533	-231.05	-287.875	-287.875
29	3842.7	3899.7	117.2	1311	308	80.4	36.4	43.143	-158.336	-220.535	-220.535
30*	3961	4023.7	115.8	2085	479	83	37.4	77.889	0	-244.1	-244.1
31	4077.6	4100.6	58.3	145	34	92.6	40.7	2.511	-28.116	-265.353	-265.353
32	4995.9	4996.8	102	2150	351	43.7	28.8	202.541	-298.638	-469.841	-469.841
33	5115.3	5116.3	62.5	2131	352	33.9	25.8	121.915	-296.334	-468.090	-468.090

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Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs. VSMQW
Duplicate 1											
1	19.4	20.5	21.9	1077	172	28.3	22.6	20.355	-452.973	-493.398	-493.398
2	99.1	100.1	21.9	1073	171	28.4	22.4	20.327	-452.354	-492.825	-492.825
3	198.6	199.6	21.9	1080	172	28.4	22.2	20.409	-451.574	-492.102	-492.102
4	298	299.1	21.9	1087	171	28.4	22.3	20.255	-451.814	-492.525	-492.525
5	541.3	558.7	82.8	824	178	30.1	22.8	13.871	6.367	-68.003	-68.003
6*	1165.4	1192.3	108.7	2385	690	39.2	25.3	58.678	0	-73.9	-73.9
7	1285.3	1307.7	61.9	55	14	50.7	28.1	2.055	-109.294	-175.117	-175.117
8	1389.4	1420.4	71.7	126	30	61.9	30.8	3.888	-160.911	-222.92	-222.92
9	1504.2	1530.3	84.6	268	63	82.4	35.6	10.12	-180.028	-240.622	-240.622
10	1569.8	1598.8	45.4	171	34	196.7	60.3	4.281	-324.465	-374.387	-374.387
11	1615.2	1648.3	50.8	1291	258	196.7	60.3	36.513	-315.299	-365.899	-365.899
12	1665.9	1685.6	46.8	940	191	196.7	60.3	24.426	-292.711	-344.979	-344.979
13	1712.5	1731.6	65.2	409	95	196.7	60.3	8.06	-153.704	-216.246	-216.246
14	1803.5	1830	91.1	453	104	114	42	16.85	-200.86	-259.916	-259.916
15	1894.6	1930.1	75	2173	492	114	42	67.808	-234.501	-291.071	-291.071
16	1969.6	2043.8	103.2	2057	467	114	42	103.075	-232.715	-289.417	-289.417
17	2072.9	2107.6	83.2	4283	1012	114	42	125.684	-247.397	-303.015	-303.015
18	2156	2182.8	76.7	1887	390	114	42	48.209	-199.916	-259.042	-259.042
19	2232.7	2276.4	84	5589	1378	114	42	180.181	-250.573	-305.956	-305.956
20	2316.8	2342.9	69.2	2086	487	114	42	59.039	-198.18	-255.582	-255.582
21	2385.9	2444.9	88.6	8342	2182	114	42	328.018	-285.025	-337.862	-337.862
22	2474.6	2488.4	59.1	2625	623	114	42	84.786	-192.542	-252.213	-252.213
23	2537	2571.1	75.7	4734	1138	114	42	150.409	-241.828	-297.95	-297.95
24	2609.4	2624.6	38.2	1523	343	114	42	33.627	-207.129	-265.722	-265.722
25	2647.6	2677.5	81.7	2318	518	114	42	80.917	-235.525	-292.02	-292.02
26	2729.3	2764	57.3	856	188	114	42	23.332	-207.69	-266.242	-266.242
27	2786.6	2810.4	61.2	360	81	114	42	15.551	-189.907	-249.773	-249.773
28*	2847.8	2883.6	82.1	2605	616	114	42	77.257	0	-244.1	-244.1
29	2930	2934.8	17.6	88	21	114	42	1.137	58.584	-199.817	-199.817
30	2947.5	2977.6	58.3	110	25	114	42	4.076	-9.503	-251.283	-251.283
31	3483.4	3484.2	31.8	1031	161	30.3	23	28.798	-307.972	-478.698	-478.698
32	3582.9	3583.9	32	1010	161	28.7	22.2	28.901	-306.033	-475.431	-475.431
Duplicate 2											
1	19.4	20.3	21.7	1008	160	28.6	22.4	18.974	-451.653	-492.185	-492.185
2	99.1	99.9	21.7	1010	159	28.6	22.4	18.947	-451.659	-492.182	-492.182
3	198.6	199.6	21.9	1002	160	28.6	22	19.034	-449.608	-490.282	-490.282
4	298	299.1	21.9	1009	159	28.6	22.5	18.884	-451.9	-492.405	-492.405
5	539.4	556.8	84.9	728	206	31.5	22.8	15.944	4.877	-69.383	-69.383
6*	1163.7	1191.9	109.3	2506	730	40.5	25	62.793	0	-73.9	-73.9
7	1283.9	1310.2	64	59	15	52.4	28.6	2.225	-123.164	-187.962	-187.962
8	1387.8	1420.8	73.8	128	30	64.3	31.3	4.195	-154.875	-217.33	-217.33
9	1502.9	1530.7	85.6	270	63	87.3	36.8	10.808	-162.821	-243.21	-243.21
10	1570.4	1599.1	43.7	162	31	214.7	64.4	4.299	-332.387	-381.724	-381.724
11	1614.1	1647.1	46.2	1296	257	214.7	64.4	39.061	-316.284	-368.81	-368.81
12	1665.5	1686.8	58.4	938	190	214.7	64.4	28.308	-290.581	-343.007	-343.007
13	1711.7	1731.8	86.5	392	91	214.7	64.4	8.498	-147.658	-210.646	-210.646
14	1802.2	1831	91.5	444	103	120.9	43.5	17.916	-196.369	-255.757	-255.757
15	1864.2	1931.8	75.9	2210	500	103.8	40.1	74.675	-235.062	-291.61	-291.61
16	1970	2045.5	102.8	2132	485	103.8	40.1	113.676	-233.199	-289.866	-289.866
17	2072.9	2109.2	83.4	4458	1054	103.8	40.1	139.046	-249.294	-304.771	-304.771
18	2156.3	2184.9	76.3	1891	390	103.8	40.1	53.9	-199.767	-258.904	-258.904
19	2232.5	2278.7	84.6	5859	1447	103.8	40.1	197.739	-252.721	-307.944	-307.944
20	2317.2	2345.4	69	2086	487	103.8	40.1	87.111	-194.394	-253.928	-253.928
21	2386.2	2447.6	90.3	8896	2320	103.8	40.1	359.808	-288.72	-342.21	-342.21
22	2476.4	2490.2	56.6	2912	692	103.8	40.1	71.633	-193.46	-253.053	-253.053
23	2533.1	2574	77.5	5093	1231	103.8	40.1	167.252	-242.903	-298.852	-298.852
24	2610.6	2626.7	38.5	1626	367	103.8	40.1	38.496	-206.389	-265.036	-265.036
25	2649.1	2679	81.7	2608	980	103.8	40.1	90.785	-233.771	-290.398	-290.398
26	2730.8	2786.1	61.7	980	216	103.8	40.1	27.698	-205.566	-264.08	-264.08
27	2786.8	2811.1	61.7	474	108	103.8	40.1	20.925	-188.821	-248.767	-248.767
28*	2848.5	2885.7	81.1	3001	711	103.8	40.1	90.028	0	-244.1	-244.1
29	2929.8	2933.5	17.1	132	32	103.8	40.1	1.747	68.531	-192.298	-192.298
30	2946.7	2976.8	59.4	142	31	103.8	40.1	5.803	-8.295	-250.37	-250.37
31	3327.3	3371	68.3	52	13	66.5	30.6	1.522	139.084	-138.967	-138.967
32	3483.4	3484.2	31.8	967	150	30.3	23.2	28.871	-300.707	-471.404	-471.404
33	3582.9	3583.7	32	945	150	28.7	22.6	26.968	-300.219	-471.036	-471.036
Duplicate 3											
1	19.4	20.5	21.7	274	45	33.1	25.3	5.21	-440.383	-481.739	-481.739
2	99.1	100.1	21.7	271	44	33.1	25.4	5.176	-444.235	-485.306	-485.306
3	198.6	199.6	21.9	271	44	33.2	25.1	5.162	-439.207	-480.65	-480.65
4	298	299.1	21.5	269	43	33.2	25.5	5.09	-444.247	-485.317	-485.317
5	504.7	528.9	103.2	3191	910	38.7	27.1	69.38	-33.686	-105.097	-105.097
6	781	793.2	58.9	181	45	36.6	28.2	3.454	-135.105	-199.021	-199.021
7*	1142.8	1171.2	102.4	2202	629	37.4	28.2	50.439	0	-73.9	-73.9
8	1561.7	1605.1	32	91	21	42.4	27.1	1.503	-159.179	-221.315	-221.315
9	1681.8	1706.5	46	76	18	51	29.3	1.564	-297.926	-349.809	-349.809
10	1744.7	1780.1	79.4	448	86	53.6	29.7	9.916	-307.734	-358.893	-358.893
11	1826.2	1844.2	49.7	285	56	61.5	31.5	5.016	-306.023	-358.382	-358.382
12	1919	1933.9	61.2	164	36	43.8	27.8	3.058	-200.104	-259.217	-259.217
13	2082.3	2098.6	51.4	194	41	39.8	26.9	3.648	-209.931	-268.317	-268.317
14	2244.2	2272.7	75	748	180	39.8	26	17.512	-217.623	-275.441	-275.441
15	2320.5	2337	33.6	58	13	73.3	34.5	0.905	-254.72	-309.796	-309.796
16	2354.8	2389.9	57.3	133	28	74.9	34.9	3.507	-277.694	-331.072	-331.072
17	2412.1	2453.2	92.6	569	122	74.9	34.9	17.075	-228.366	-285.39	-285.39
18	2564.8	2591.2	101.8	1205	262	40.9	26.6	32.243	-215.449	-273.427	-273.427
19	2705.3	2729.7	74.2	546	120	44.1	27.6	11.808	-204.703	-263.475	-263.475
20	2849.1	2892.8	110.8	1598	355	44.6	27.4	48.446	-204.861	-263.621	-263.621
21	2991	3018.2	87.8	638	141	52.7	27.9	14.213	-168.651	-230.273	-230.273
22	3125.8	3184.5	139.2	2443	654	46.2	28	93.861	-203.69	-282.537	-282.537
23	3285.6	3296.3	80.5	469	102	67.6	33.2	9.502	-212.265	-270.479	-270.479
24	3383.1	3428.6	95.3	1283	285	67.6	30.3	39.217	-208.885	-267.348	-267.348
25	3479	3500.1	42.4	141	29	57	48.4	1.99	-302.482	-354.029	-354.029
26	3521.4	3534	36.2	97	22	132.8	48.4	0.532	-231.789	-288.56	-288.56
27	3558.4	3564.1	53.5	422	86	91.1	38.7	8.883	-262.239	-316.759	-316.759
28	3610.9	3619.3	22.2	71	16	91.1	38.7	1.088	-250.478	-305.868	-305.868
29	3633	3649.8	38.2	228	51	91.1	38.7	4.073	-200.002	-259.121	-259.121
30	3743.8	3785.3	63.7	237	53	80.1	36.6	5.06	-212.245	-270.46	-270.46
31	3844.6	3872.6	46.6	57	14	77	35.9	1.155	-112.118	-177.733	-177.733
32*	3906.6	4027.2	121.2	2332	537	85.6	38.8	86.842	0	-244.1	-244.1
33	4995.9	4996.8	101.2	183	29	49.4	31.1	16.123	-348.512	-507.541	-507.541
34	5115.3	5116.3	61.7	180	31	33	25.2	10.489	-275.735	-452.528	-452.528
Duplicate 4											
1	19.4	20.3	21.5	177	30	33.1					

7*	1144.1	1171	100.9	2127	607	37.2	26.4	48.104	0	-73.9	-73.9
8	1592	1605.1	31.8	83	15	42.3	27.5	1.373	-190.274	-250.113	-250.113
9	1681.6	1706.3	46	70	15	49.7	28.6	1.447	-249.89	-305.323	-305.323
10	1744.3	1779.2	79.4	416	80	52.1	29.2	9.14	-299.945	-351.679	-351.679
11	1825.8	1843.6	50	264	53	58.9	30.4	4.662	-282.946	-335.936	-335.936
12	1918.8	1933.5	60.4	150	34	42.9	27.5	2.808	-192.385	-252.068	-252.068
13	2082.1	2098.2	51.2	169	38	39.4	26.7	3.355	-198.562	-257.788	-257.788
14	2243.8	2271.4	74.6	698	149	39.2	26.6	16.181	-227.092	-284.21	-284.21
15	2319.7	2336.2	33.9	54	13	69.8	33.5	0.848	-215.399	-273.381	-273.381
16	2354.2	2389.1	56.6	122	26	72	34.2	3.241	-271.547	-325.38	-325.38
17	2411.2	2451.8	92.8	522	112	81.5	36.4	14.694	-225.33	-282.578	-282.578
18	2554.4	2589.7	101.6	1133	245	40.6	28.8	29.794	-218.083	-275.866	-275.866
19	2704.7	2728.7	74	511	113	43.7	27.4	10.839	-199.085	-258.272	-258.272
20	2848.5	2890.9	110.4	1512	335	44.4	27.3	44.778	-203.323	-262.198	-262.198
21	2990.6	3016.9	86.9	600	132	52.3	29.5	13.224	-201.801	-260.787	-260.787
22	3125.4	3182.2	138.8	2331	528	46.5	28.1	87.85	-202.824	-261.735	-261.735
23	3264.8	3285.3	80.9	450	98	67.3	33.2	9.163	-208.159	-266.676	-266.676
24	3382.5	3427.4	95.1	1247	276	58.1	30.6	37.671	-206.645	-265.274	-265.274
25	3478.4	3499.1	42.4	132	27	130.1	48	1.851	-308.387	-359.497	-359.497
26	3520.8	3533.6	36.4	100	22	130.1	48	0.648	-214.937	-272.953	-272.953
27	3558	3583.5	52.3	423	86	95.9	40.6	8.845	-274.575	-328.183	-328.183
28	3632.8	3650.4	40.3	262	59	107.9	42.1	4.447	-173.317	-234.409	-234.409
29	3743.4	3765.1	64.4	235	53	79.7	35.9	5.017	-184.229	-244.514	-244.514
30	3844.6	3873.8	48.7	100	24	75.4	35.8	2.04	-145.075	-208.254	-208.254
31*	3966.4	4024.1	119.5	2158	496	85.5	38.9	77.182	0	-244.1	-244.1
32	4965.7	4996.8	101.2	117	19	48.8	31.1	10.131	-355.829	-513.071	-513.071
33	5115.3	5116.1	61.4	119	21	32.8	25.4	6.894	-248.595	-432.013	-432.013

Triplicate 1

1	18.8	20.5	22.8	1029	172	258	93.3	20.14	-421.232	-464.003	-464.003
2	99.1	100.1	22.2	1028	173	258.4	92.5	20.152	-418.608	-461.573	-461.573
3	197.9	199.8	22.6	1026	172	256.7	92.6	20.189	-419.288	-462.203	-462.203
4	298.2	299.3	22.2	1025	171	256.7	92.8	20.055	-420.018	-462.879	-462.879
5	368	372.4	26.1	8747	1832	256.3	92.7	25.155	-397.619	-442.135	-442.135
6*	950.1	973.7	46.6	7894	2151	281.2	93.6	86.8	0	-73.9	-73.9
7	1072	1076.1	17.8	64	16	270.7	95.5	0.429	-27.469	-96.339	-96.339
8	1198	1203.8	11.1	91	23	276.9	97.7	0.468	-91.929	-159.035	-159.035
9	1209.1	1213.2	20.9	73	17	276.9	97.7	0.468	-189.524	-249.419	-249.419
10	1338.4	1346.6	26.8	25	17	276.9	97.7	3.236	-157.72	-219.965	-219.965
11	1365.2	1374	22.8	72	17	274	97.1	0.949	-189.456	-249.355	-249.355
12	1392.1	1409.9	38	205	43	279.2	98	2.796	-245.88	-301.609	-301.609
13	1446.7	1478.3	43.7	1274	241	287.5	99	13.441	-268.151	-322.234	-322.234
14	1490.4	1496.9	21.7	241	53	287.5	99	2.283	-211.789	-270.037	-270.037
15	1519.8	1533.9	33.4	972	190	299.1	101.1	8.433	-244.73	-300.544	-300.544
16	1601.8	1609.9	23.4	89	22	275.3	96.3	0.873	-110.929	-176.631	-176.631
17	1640.9	1652.8	30.5	475	111	270.9	95.7	4.962	-150.042	-212.854	-212.854
18	1797.6	1810.8	34.7	458	109	279.8	97.8	5.353	-150.721	-213.483	-213.483
19	1848.2	1859.5	28.8	125	28	274.1	95.9	1.579	-187.332	-247.388	-247.388
20	1955.6	1982.2	37.6	2061	426	275.4	96.4	28.147	-191.218	-250.987	-250.987
21	1993.2	2003.9	29.1	176	38	275.4	96.4	3.067	-220.418	-278.029	-278.029
22	2022.3	2038	24.9	226	50	275.4	96.4	3.855	-197.231	-256.556	-256.556
23	2047.2	2060.3	33.6	393	85	275.4	96.4	5.483	-214.417	-272.472	-272.472
24	2094.6	2120.3	29.7	2176	437	282.2	97	24.898	-187.422	-228.949	-228.949
25	2124.3	2127.4	21.3	1004	218	282.2	97	7.264	-241.036	-297.124	-297.124
26	2259.9	2296.1	51.4	3156	643	268.8	94.8	52.688	-196.371	-255.759	-255.759
27	2409.8	2433.6	41	1532	321	279.1	97.5	19.38	-169.746	-231.102	-231.102
28	2481.2	2499	42.2	68	15	282	97.1	1.331	-185.42	-245.617	-245.617
29	2552.1	2596.2	56	3831	806	272.8	95.2	78.914	-190.386	-250.217	-250.217
30	2608.5	2615.2	21.1	86	20	313.6	102.3	0.747	-61.9	-131.226	-131.226
31	2694.8	2721.8	46.6	1722	358	285	97.4	23.877	-164.327	-226.083	-226.083
32	2827.8	2886.5	65.8	4735	1044	279.4	96.3	144.236	-189.378	-249.283	-249.283
33	2893.6	2898.2	16.9	347	76	279.4	96.3	2.88	-203.103	-261.994	-261.994
34	2910.5	2943.8	48.5	102	25	279.4	96.3	2.538	-129.068	-193.43	-193.43
35	2964.5	2990.6	39.9	1466	307	292.3	99.5	17.35	-165.606	-227.268	-227.268
36	3033.6	3050.4	23.8	152	34	294.6	100	1.469	-207.073	-265.67	-265.67
37	3094.2	3138.1	49.1	3280	873	309.7	103	66.69	-178.979	-239.652	-239.652
38	3143.4	3146.3	8.2	692	139	309.7	103	4.157	-283.062	-336.044	-336.044
39	3151.5	3152.3	18.4	216	45	309.7	103	1.34	-274.875	-328.461	-328.461
40	3214.6	3239.1	45.1	1510	339	308.7	102.2	23.411	-205.708	-264.407	-264.407
41	3259.8	3276.1	30.3	274	60	308.7	102.2	2.732	-214.586	-272.629	-272.629
42	3345.3	3364.9	30.9	1063	215	280.8	95.4	9.757	-144.316	-207.551	-207.551
43	3378.9	3390.8	24.7	191	45	288.8	96.4	1.782	-126.728	-191.263	-191.263
44	3406.3	3428.6	30.9	724	144	306.3	101.5	8.41	-184.329	-244.607	-244.607
45	3437.2	3443.1	16.3	68	15	306.3	101.5	0.463	-267.591	-321.716	-321.716
46	3464.8	3474.8	22.6	106	26	287.8	96.9	0.803	-72.09	-140.683	-140.683
47	3519.1	3529	20.7	125	29	290.3	98.2	0.976	-177.406	-238.196	-238.196
48	3580.6	3592.9	28	232	55	301	100.1	1.464	-81.57	-149.442	-149.442
49	3609.6	3623.9	26.8	160	38	276.5	95.5	1.66	-155.336	-217.757	-217.757
50	3638.0	3648.5	25.9	121	30	294.5	98.5	1.715	-143.013	-206.344	-206.344
51	3660	3671.4	21.3	58	14	282.8	96.5	0.461	-143.017	-206.348	-206.348
52	3832.9	3845	24.9	91	23	280.5	95.2	0.937	-84.536	-152.188	-152.188
53	3857.3	3871.5	25.5	96	23	280.5	95.2	1.336	-123.227	-188.02	-188.02
54	4069.9	4082.4	22.6	63	15	287.5	97.1	0.748	-123.069	-187.875	-187.875
55	4285.1	4300.4	25.3	55	14	288.8	97.3	0.714	-101.371	-167.779	-167.779
56	4570.2	4587.1	33	64	17	283.9	96.2	1.101	-88.647	-155.996	-155.996
57	4996.6	4997.8	101.4	958	160	258.9	93.2	94.393	-419.602	-462.493	-462.493
58	5116.1	5117.4	61.9	950	159	258.4	93.3	56.376	-419.864	-462.736	-462.736

Triplicate 2

1	19.4	20.7	21.9	944	158	258	93.3	18.496	-420.337	-463.174	-463.174
2	99.1	100.3	22.8	942	159	258	91.9	18.451	-413.621	-456.954	-456.954
3	198.6	199.8	21.9	941	157	258.4	93.3	18.523	-419.773	-462.652	-462.652
4	298	299.3	21.9	941	157	258.2	93.2	18.398	-420.274	-463.116	-463.116
5	368.7	371.8	18.8	6020	850	258.3	93.5	13.789	-563.978	-596.2	-596.2
6*	949.7	972.3	46	7788	2109	264.2	94.5	85.758	0	-73.9	-73.9
7	1068	1074.7	9.6	69	18	271.5	95.5	0.283	47.799	-29.633	-29.633
8	1089.3	1094.1	13	52	14	274.2	97	0.202	-33.864	-105.261	-105.261
9	1196.3	1202.2	10.9	134	35	279.9	98.3	0.599	-58.716	-128.277	-128.277
10	1207.2	1211.4	14.8	93	21	278.7	98.3	0.532	-203.582	-262.438	-262.438
11	1337.2	1344.3	26.1	262	66	279.9	97.8	3.472	-147.65	-210.639	-210.639
12	1363.3	1371.9	27	88	21	276.7	97.8	1.067	-162.245	-224.155	-224.155
13	1390.3	1407.6	37.8	248	53	278.5	97.8	3.213	-231.558	-288.345	-288.345
14	1444.6	1450.5	16.7	60	14	293.5	100.3	0.636	-160.243	-222.301	-222.301
15	1481.3	1476	21.4	1297	242	293.5	100.3	13.467	-276.89</		

1622 CONT

28	2256.2	2294.8	57.9	3295	865	270.5	95.3	56.269	-198.475	-257.708	-257.708
29	2406.8	2431.5	45.4	1534	321	284.2	98.1	20.496	-167.317	-228.853	-228.853
30	2480	2497.8	49.1	70	16	284.1	97.4	1.495	-161.294	-223.275	-223.275
31	2548.8	2583.9	58.3	3747	833	276.5	96	83.038	-188.46	-248.433	-248.433
32	2607.1	2614.4	21.3	127	29	276.5	96	1.67	-216.294	-274.21	-274.21
33	2692.1	2719.9	46.8	1690	355	289.2	98.8	25.05	-165.471	-227.143	-227.143
34	2827.1	2886.7	65.8	4863	1085	282.7	97.3	148.248	-188.072	-248.074	-248.074
35	2893	2897.4	16.1	368	81	282.7	97.3	2.939	-200.065	-259.18	-259.18
36	2909.1	2942.1	46.4	104	25	282.7	97.3	2.567	-126.12	-190.7	-190.7
37	2963.8	2989.3	38.9	1512	312	296.5	100.9	18.725	-158.667	-226.305	-226.305
38	3035.1	3049.3	21.1	152	34	299.7	100.9	1.494	-163.603	-225.413	-225.413
39	3091.9	3137.1	51	3395	691	319.6	103.5	70.391	-173.794	-234.85	-234.85
40	3142.9	3145.4	7.5	727	141	319.6	103.5	3.771	-330.509	-330.509	-330.509
41	3168.9	3177.6	14.8	58	13	305.5	101.8	0.486	-160.366	-222.415	-222.415
42	3195.2	3201.7	14.2	50	14	302.6	101.5	0.365	-141.002	-204.482	-204.482
43	3210.2	3237.8	47.4	1575	350	314.1	104	24.797	-209.223	-267.661	-267.661
44	3257.7	3274.6	30.7	284	61	314.1	104	2.881	-240.68	-296.794	-296.794
45	3344	3363	32.4	1095	226	282.9	96.8	10.398	-155.105	-217.543	-217.543
46	3377.4	3389.6	24.7	202	47	291.5	97.4	1.904	-136.014	-199.862	-199.862
47	3404.4	3427.4	31.1	750	149	309.9	102.3	8.934	-185.842	-248.009	-248.009
48	3435.5	3441.8	16.9	74	16	309.9	102.3	0.499	-273.057	-326.778	-326.778
49	3463.3	3473.2	22.2	110	26	290.3	97.6	0.862	-107.209	-173.186	-173.186
50	3518.3	3527.5	20.3	130	30	293.9	98.7	1.021	-159.805	-221.896	-221.896
51	3579.5	3591	27.4	240	58	305.2	101.3	1.731	-110.653	-176.375	-176.375
52	3609.4	3621.8	24	169	41	282	95.8	1.731	-131.432	-195.619	-195.619
53	3635.6	3647.7	27.4	127	30	298.9	99.6	1.814	-147.862	-210.835	-210.835
54	3652.9	3673.4	21.1	67	16	298.9	99.6	0.724	-142.561	-205.926	-205.926
55	3692.8	3703.5	24.2	54	13	292.3	98.1	0.403	-68.496	-137.334	-137.334
56	3606.5	3815.5	21.5	64	16	286.9	97	0.495	-110.915	-176.618	-176.618
57	3831.4	3843.5	24.2	94	25	284.3	94.5	1.002	18.231	-57.017	-57.017
58	3856.7	3869.4	24.9	91	22	295.9	98.2	1.141	-81.102	-149.009	-149.009
59	4044.1	4056.1	21.9	51	13	281.7	95.8	0.505	-122.301	-187.163	-187.163
60	4066.9	4079.5	22.4	69	17	288.3	97	0.791	-84.834	-152.464	-152.464
61	4282.4	4296	24.9	56	14	294.2	98.3	0.73	-88.189	-155.572	-155.572
62	4565.2	4582.7	33.9	65	16	288.3	97.2	1.11	-103.989	-170.205	-170.205
63	4996.8	4997.8	101.4	880	147	257.8	92.9	86.889	-419.38	-462.288	-462.288
64	5115.7	5140.4	62.7	872	146	260	93.3	51.915	-419.782	-462.86	-462.86

Triplicate 3

1	19.4	20.7	22.2	866	144	259.5	93.2	16.967	-419.413	-462.318	-462.318
2	99.1	100.3	23	865	144	258.5	93.1	16.952	-419.5	-462.399	-462.399
3	198.6	210.7	22.4	864	144	257.7	92.8	17.043	-418.699	-461.657	-461.657
4	298.2	299.3	21.9	863	144	258.4	93	16.897	-419.698	-462.582	-462.582
5	367.6	371.4	18.2	2867	257	257.4	92.8	6.214	-671.518	-695.793	-695.793
6	911.4	917.7	15.5	54	15	265	94.3	0.285	99.911	18.627	18.627
7*	947.8	971.6	44.5	7995	2182	264.8	94.4	89.738	0	-73.9	-73.9
8	1069.7	1073.6	7.1	77	20	273.6	96.7	0.287	-62.817	-132.075	-132.075
9	1088.9	1093.1	13.4	55	14	275.8	97.1	0.212	10.59	-64.093	-64.093
10	1194.6	1201.1	11.5	151	39	280.7	98.5	0.67	-85.1	-134.189	-134.189
11	1206.1	1210.3	16.9	102	23	280.7	98.5	0.587	-236.807	-293.207	-293.207
12	1334.9	1343.7	27.6	306	75	280.1	97.9	3.852	-154.857	-217.313	-217.313
13	1362.5	1371.2	25.5	96	24	280.1	97.9	1.138	-149.148	-212.026	-212.026
14	1398	1407.2	39.1	280	59	280.1	97.9	3.571	-242.491	-298.471	-298.471
15	1443.4	1449.6	16.7	73	18	293.8	100.2	0.742	-166.674	-228.257	-228.257
16	1460.3	1476.4	27.6	1426	252	326.1	107.5	13.906	-285.075	-337.908	-337.908
17	1487.9	1494.1	22.2	235	53	326.1	107.5	2.111	-207.317	-265.896	-265.896
18	1518.2	1532	41.8	1116	206	312.8	104.4	9.527	-256.635	-311.57	-311.57
19	1598.8	1606.4	29.9	96	25	278.6	97.1	1.088	-95.866	-162.681	-162.681
20	1638.1	1649.6	43.7	460	110	274.3	96.6	6.151	-153.147	-215.73	-215.73
21	1794.7	1807.4	41.4	440	105	286.4	98.7	6.341	-143.291	-206.602	-206.602
22	1844.2	1855.9	40.1	123	28	280.5	97.2	1.881	-200.309	-259.406	-259.406
23	1953.1	1980.5	38.7	2156	448	284.8	98.4	9.236	-193.231	-252.851	-252.851
24	1991.8	1998.9	28.4	175	39	284.8	98.4	3.386	-216.482	-274.384	-274.384
25	2020.2	2058.2	66.7	381	84	284.8	98.4	10.689	-210.904	-269.219	-269.219
26	2088.7	2118.8	33.9	2443	497	288.5	98.2	29.316	-172.249	-233.42	-233.42
27	2258.6	2295.2	54.5	3433	692	273.7	95.5	60.936	-197.901	-257.176	-257.176
28	2406	2431.3	44.5	1603	345	283.8	98	22.38	-168.513	-229.96	-229.96
29	2481.9	2495.5	42.8	72	16	286	97.7	1.532	-165.744	-227.396	-227.396
30	2548.3	2595.8	58.7	3699	836	275.1	95.8	88.537	-186.478	-246.598	-246.598
31	2607.1	2613.5	20.5	147	33	275.1	95.8	1.832	-207.836	-266.377	-266.377
32	2627.5	2631.7	15	57	13	275.1	95.8	0.637	-197.795	-257.078	-257.078
33	2690	2719.3	50.6	1727	370	290.1	98.6	27.182	-161.545	-223.507	-223.507
34	2780.1	2796.2	39.7	53	13	295.1	100	0.879	-147.631	-210.621	-210.621
35	2825.7	2888.2	68.1	5118	1144	286.4	98	161.369	-189.239	-248.154	-248.154
36	2893.8	2898	15.5	410	91	286.4	98	3.202	-201.23	-260.259	-260.259
37	2909.3	2941.7	51.8	110	27	286.4	98	2.757	-120.85	-185.819	-185.819
38	2953.4	2990	41	1563	332	290.2	100.9	20.443	-166.547	-228.14	-228.14
39	3031.3	3049.3	25.9	163	36	300.4	101.4	1.728	-198.928	-258.127	-258.127
40	3092.6	3138.3	50.8	3552	729	329.1	107.3	76.014	-178.43	-239.144	-239.144
41	3143.4	3145.4	25.3	758	149	329.1	107.3	5.472	-278.109	-331.457	-331.457
42	3169.3	3177.4	14.8	62	15	308.7	102.5	0.509	-160.216	-222.276	-222.276
43	3195.4	3201.9	14.4	60	14	303.3	101.6	0.427	-150.583	-213.365	-213.365
44	3211.9	3237.8	46.4	1662	369	314.6	103.6	27.353	-208.13	-268.65	-268.65
45	3258.3	3275.4	30.1	311	67	314.6	103.6	3.307	-221.56	-279.087	-279.087
46	3343.2	3364.1	33.6	1173	247	283.3	95.4	11.468	-141.591	-204.999	-204.999
47	3376.8	3390.2	28.6	234	54	283.3	95.4	2.468	-145.616	-208.755	-208.755
48	3405.4	3428.4	31.3	849	168	283.3	95.4	10.849	-178.913	-239.592	-239.592
49	3436.8	3442.2	16.5	116	26	283.3	95.4	0.509	-173.158	-234.261	-234.261
50	3463.3	3473.8	21.5	117	29	294.3	98.7	0.924	-132.962	-197.036	-197.036
51	3518.9	3529	20.7	146	33	297.5	99.6	1.111	-170.935	-232.202	-232.202
52	3580.6	3592.3	25.3	265	63	305.6	101.2	1.821	-100.827	-167.276	-167.276
53	3609.4	3623.2	26.3	181	44	284.8	96.4	1.9	-127.655	-192.121	-192.121
54	3637.2	3647.9	27.2	140	33	300	99.9	2.061	-158.306	-220.507	-220.507
55	3664.4	3675.1	20.3	77	18	300	99.9	0.849	-166.001	-227.633	-227.633
56	3694.7	3704.5	21.7	60	15	295.9	99.1	0.424	-98.919	-165.509	-165.509
57	3807.6	3816.8	23.8	67	17	288.4	97.3	0.529	-93.999	-160.952	-160.952
58	3831.8	3845.2	25.9	106	26	284	95.7	1.578	-81.807	-149.661	-149.661
59	3857.7	3870.9	24	113	27	284	95.7	1.578	-120.173	-185.192	-185.192
60	4045.4	4057.9	23.2	56	27	282.3	95.7	0.578	-82.75	-150.535	-150.535
61	4069.2	4082	21.9	78	19	289.9	97.3	0.852	-107.672	-173.615	-173.615
62	4260	4272	24.2	50	13	290	97.1	0.556	-21.381	-93.701	-93.701
63	4285.3	4299.1	24.9	63	16	293.5	97.8	0.846	-63.238	-132.465	-132

1622 CONT

C16	950.1	959.7	947.8
C23	1982.2	1980.5	1980.5
C25	2296.1	2294.8	2295.2
C27	2596.2	2593.9	2595.8
C29	2886.5	2886.7	2888.2
C36	4033	4033	4033

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Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area.all (Vs)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs. VSMOW	
Duplicate 1												
1	19.4	20.3	21.7	637	100	28.5	21.5	12.048	-450.542	-491.147	-491.147	
2	99.1	99.9	21.7	643	100	28.5	22.1	12.034	-454.741	-495.035	-495.035	
3	198.6	199.6	21.9	633	100	28.5	21.9	12.084	-452.913	-493.343	-493.343	
4	298	299.1	21.7	637	99	28.5	22	12.001	-453.823	-494.186	-494.186	
5	441.6	456.5	85.3	1666	457	30.1	22.2	30.252	-33.411	-104.842	-104.842	
6*	1075.9	1098.5	96.3	2012	562	34.7	23.2	40.816	0	-73.9	-73.9	
7	1578.8	1585.9	42.2	55	12	37.8	24.1	0.845	-238.251	-295.47	-295.47	
8	1724.7	1731.4	30.1	52	13	49	35	23.2	-114.234	-179.692	-179.692	
9	1817	1826.5	54.5	221	49	35	23.1	0.743	-191.267	-251.032	-251.032	
10	1902.5	1913.4	32	108	24	41.6	24.8	1.532	-205.466	-264.182	-264.182	
11	1991.6	2002.6	62.3	366	80	36.8	23.4	5.949	-190.29	-250.128	-250.128	
12	2074.5	2082.5	42.8	129	29	38.6	24	1.82	-186.593	-246.703	-246.703	
13	2154	2169.6	77.3	851	183	38.2	24	15.251	-212.341	-270.549	-270.549	
14	2231.9	2241.9	49.5	314	67	46.2	25.9	4.785	-219.268	-276.964	-276.964	
15	2305.7	2326.6	58.5	1566	337	42.8	24.9	30.265	-222.024	-279.516	-279.516	
16	2364.2	2366.1	15.5	78	19	42.8	24.9	0.869	-151.378	-214.091	-214.091	
17	2379.7	2388.9	66.9	321	70	42.8	24.9	5.396	-215.277	-273.268	-273.268	
18	2448.2	2463.5	65.6	810	174	46.4	25.6	14.462	-211.498	-269.788	-269.788	
19	2514.3	2522.8	39.7	97	22	62	29.4	1.174	-231.841	-288.508	-288.508	
20	2559.6	2567.1	21.9	68	15	54.1	27.1	0.789	-225.277	-282.529	-282.529	
21	2581.6	2589.1	34.3	163	36	54.1	27.1	2.422	-185.033	-245.257	-245.257	
22	2644.5	2652	20.3	98	23	53	27.2	1.129	-189.826	-249.698	-249.698	
23	2664.8	2668.9	33	52	12	53	27.2	0.817	-193.257	-252.876	-252.876	
24	2705.3	2713.4	34.5	80	19	55.5	27.8	1.334	-191.912	-251.63	-251.63	
25*	2770.9	2809	83.8	2712	618	57.3	28	72.717	0	-244.1	-244.1	
26	3482.8	3483.8	31.8	609	95	28.8	22.2	17.292	-312.269	-480.144	-480.144	
27	3582.3	3583.3	32	612	95	28.4	21.9	17.343	-311.219	-479.351	-479.351	
Duplicate 2												
1	19.4	20.3	21.7	616	95	28.5	21.7	11.427	-450.035	-490.877	-490.877	
2	99.1	99.9	21.7	613	94	28.5	22.1	11.415	-452.343	-492.815	-492.815	
3	198.6	199.4	21.7	614	94	28.5	22.3	11.462	-454.218	-494.551	-494.551	
4	298	298.9	21.7	613	94	28.5	22	11.383	-457.733	-493.176	-493.176	
5	441.2	457.1	90.3	2055	564	30.1	22.4	38.056	-33.733	-105.138	-105.138	
6*	1074.9	1099.1	99.9	2272	638	35	23.7	47.888	0	-73.9	-73.9	
7	1577.5	1585.1	42.8	53	12	37.7	24.3	0.825	-232.742	-289.443	-289.443	-6.027
8	1723.2	1730.7	30.9	52	12	35.4	23.9	0.737	-205.856	-264.543	-264.543	84.851
9	1814.5	1825.6	56.2	216	48	35	23.1	3.466	-169.645	-231.008	-231.008	-20.024
10	1901.5	1912.8	32.4	107	24	41.6	24.9	1.522	-201.877	-260.858	-260.858	-3.324
11	1988.8	2002	64.2	357	79	36.7	23.5	5.869	-182.755	-243.15	-243.15	-6.978
12	2072.7	2081.6	43.7	126	28	38.6	24.4	1.886	-197.309	-256.628	-256.628	9.925
13	2150.8	2168.8	78	826	178	38.3	24.2	15.009	-210.039	-268.418	-268.418	-2.131
14	2229.6	2241.1	51.2	305	66	47.1	26	4.641	-201.274	-260.3	-260.3	-16.864
15	2302.6	2325.5	61.4	1518	327	43.1	25.1	29.887	-218.412	-276.172	-276.172	-3.344
16	2364	2365.7	13.8	73	18	43.1	25.1	0.75	-133.629	-197.854	-197.854	-16.437
17	2377.8	2388.2	66	312	68	43.1	25.1	5.289	-202.636	-261.561	-261.561	-11.707
18	2445.1	2462.4	67.9	785	169	47.2	25.8	14.188	-206.978	-265.582	-265.582	-4.186
19	2513.4	2522.2	39.9	95	21	61.7	29.4	1.143	-200.29	-259.389	-259.389	-29.219
20	2559.9	2566.5	23.4	66	14	53.5	27.6	0.764	-260.393	-315.05	-315.05	32.521
21	2580.7	2588.5	34.3	138	30	73.6	31.9	1.639	-186.983	-247.065	-247.065	1.808
22	2643	2651.6	21.5	108	25	52.7	27.3	1.24	-188.443	-248.417	-248.417	-1.281
23	2704.5	2713	34.3	76	18	52.4	27.2	1.177	-152.205	-214.857	-214.857	-38.019
24*	2767.4	2810.6	120.6	2945	676	56	28.3	85.433	0	-244.1	-244.1	0
25	3482.8	3483.6	31.8	588	90	28.7	22.5	16.406	-312.169	-480.069	-480.069	
26	3582.3	3583.1	31.8	580	90	28.4	22.3	16.456	-310.679	-478.942	-478.942	
NEW												
Triplicate 1												
1	19	20.5	22.2	936	159	234.5	94.6	18.272	-438.584	-480.999	-480.999	
2	98.2	100.1	22.8	935	159	233.7	94.3	18.279	-438.752	-480.228	-480.228	
3	198.6	199.6	21.9	933	159	235.3	93.2	18.317	-434.208	-476.02	-476.02	
4	298	299.3	22.2	932	157	234.3	94.5	18.212	-430.134	-480.582	-480.582	
5*	922.3	939.2	38.5	5290	1383	248.9	97.5	43.194	0	-73.9	-73.9	
6	1042.9	1048.8	19.4	88	22	248.1	98	0.633	-130.865	-195.094	-195.094	
7	1064	1069	13.8	71	20	254.4	99.3	0.31	0.036	-73.866	-73.866	
8	1172.1	1178.8	13.4	95	25	251.2	98.6	0.499	-96.726	-163.478	-163.478	
9	1314.6	1321.5	15	179	44	245.8	96.5	0.92	-119.758	-184.808	-184.808	
10	1339.5	1345.3	10.5	51	14	248.3	97	0.245	28.3	-47.691	-47.691	
11	1367.5	1377.1	16.5	263	58	245.8	96.8	1.51	-225.226	-282.482	-282.482	
12	1384	1388.4	14.4	118	24	245.8	96.8	0.7	-274.75	-328.346	-328.346	
13	1462.8	1472	23	109	26	242.8	96.3	0.685	-177.756	-238.52	-238.52	
14	1499.8	1509.6	25.5	479	96	245.7	96.6	0.685	-245.906	-301.634	-301.634	
15	1620.6	1628.5	20.1	217	51	239.3	94.5	1.303	-140.356	-203.884	-203.884	
16	1777.8	1786.7	22.6	233	55	240.1	95.4	1.506	-175.409	-236.346	-236.346	
17	1935.3	1948.7	30.7	771	198	238.6	94.5	5.653	-190.01	-249.868	-249.868	
18	2025	2032.7	16.5	78	19	244.3	95.8	0.509	-186.826	-246.919	-246.919	
19	2091	2099.8	23.8	288	65	248.8	97.6	1.829	-206.9	-265.51	-265.51	
20	2240.5	2256.4	29.3	804	167	239	93.8	6.308	-181.803	-242.267	-242.267	
21	2388	2399.1	26.3	212	49	243.4	95.7	1.5	-192.447	-252.125	-252.125	
22	2533.3	2550	29.5	964	196	240.1	94.8	8.553	-205.914	-264.597	-264.597	
23	2670	2683.6	35.3	284	67	246.3	94.3	1.995	-120.053	-185.081	-185.081	
24	2806.7	2827.4	34.9	1139	236	245.8	95.7	10.837	-209.747	-269.147	-269.147	
25	2940.8	2951.3	26.8	194	45	248.8	96.4	1.408	-203.214	-262.097	-262.097	
26	3070	3084.2	28.2	490	108	244.7	95.2	3.785	-195.874	-255.299	-255.299	
27	3100.1	3108.2	14	60	14	253	96	0.448	-161.118	-223.112	-223.112	
28	3198.2	3206.5	23.6	237	52	243.9	95.1	1.867	-245.704	-301.446	-301.446	
29	3330	3337.5	19.2	70	17	242.8	93.9	0.507	-147.008	-210.045	-210.045	
30	3392.5	3402.7	22.6	70	18	243.3	92.5	0.601	19.617	-55.733	-55.733	
31	4996.4	4997.6	101.6	869	147	232.8	94.3	85.762	-440.35	-481.708	-481.708	
32	5115.7	5116.9	62.1	865	146	232.3	94.1	51.397	-439.807	-481.206	-481.206	
Triplicate 2												
1	19.4	20.5	21.7	844	143	235.1	94.5	16.509	-439.604	-481.017	-481.017	
2	99.1	100.3	21.7	844	144	234.1	92.6	16.499	-432.866	-474.778	-474.778	
3	198.3	199.8	22.4	842	142	235.4	94.2	16.553	-438.246	-479.76	-479.76	
4	297.2	299.3	22.8	842	142	234.3	94.7	16.472	-441.092	-482.395	-482.395	
5	380.8	386.6	11.3	2823	716	235	94.7	10.157	-34.748	-106.08	-106.08	
6	392.1	394.8	13	399	74	235	94.7	3.932	-54.382	-124.263	-124.263	
7	405	422.2	38.2	278	80	235	94.7	5.639	-104.544	-104.544	-104.544	
8*	978.3	988.8	32.4	2749	680	237.8	95.4	16.072	0	-73.9	-73.9	
9	1555.4	1561	15.9	66	13	236.9	94.9	0.328	-198.742	-257.955	-257.955	
10	1988.6	1998.2	20.5	183	42	235.4	94.5	1.134	-194.995	-254.485	-254.485	
11	2144.8	2152.5	19.6	63	16	240.2	95.2	0.404	-152.769	-215.379	-215.379	
12	2296.7	2305										

21	4996.6	4997.6	101.8	786	133	235.3	94.3	77.443	-440.091	-481.468	-481.468
22	5115.1	5117.2	62.9	782	132	233.9	94.3	46.435	-441.133	-482.433	-482.433
Triplicate 3											
1	19.4	26.1	22.4	775	131	235.9	94.7	15.197	-427.975	-470.247	-470.247
2	98.9	100.3	21.9	776	131	234.9	94.6	15.183	-428.489	-470.724	-470.724
3	198.6	199.8	23.4	773	130	235.3	94.8	15.234	-428.726	-470.943	-470.943
4	298.2	299.3	22.4	772	130	234.9	94.9	15.12	-429.307	-471.481	-471.481
5	412.8	416.3	16.3	73	20	235.2	94.8	0.419	-8.899	-82.142	-82.142
6*	1009.7	1016.6	17.1	275	74	240.1	96	1.073	0	-73.9	-73.9
7	1132.2	1136.8	19.6	54	14	240.5	96	0.379	-109.856	-175.638	-175.638
8	1259.4	1266.3	13.8	75	18	245.6	97.5	0.384	-119.005	-184.11	-184.11
9	1402.6	1409.1	16.1	193	46	245	96.8	0.949	-113.344	-178.867	-178.867
10	1426.8	1432.7	10.4	56	15	246.4	97.3	0.265	-113.981	-178.867	-178.867
11	1456.3	1464.5	14.6	262	58	243.9	95.1	1.402	-114.631	-178.867	-178.867
12	1470.9	1475.3	15.7	120	26	243.9	95.1	0.963	-115.664	-178.867	-178.867
13	1551.6	1559.3	24.2	157	37	245.5	96.5	0.88	-115.666	-178.867	-178.867
14	1587.4	1596.8	23.4	517	103	248.4	97.7	2.866	-118.074	-183.248	-183.248
15	1704.6	1716.5	23.2	363	82	241.9	96	2.088	-233.585	-290.224	-290.224
16	1865.7	1875.4	24	432	98	242	96.2	2.715	-159.778	-221.87	-221.87
17	2023.1	2039.6	30.1	1269	250	241.8	95.8	10.667	-158.809	-221.899	-221.899
18	2111.9	2120.7	16.7	165	36	246.8	96.5	1	-183.281	-243.636	-243.636
19	2164	2171.1	14	95	22	246.3	96.4	0.534	-217.54	-275.364	-275.364
20	2178	2189.3	23.6	581	128	246.3	96.4	4.058	-181.591	-242.071	-242.071
21	2327.4	2348.7	34.9	1445	283	241.2	95.1	13.647	-170.475	-231.777	-231.777
22	2475.6	2489.2	29.5	482	109	243.5	95.3	3.84	-145.479	-242.894	-242.894
23	2619.4	2646.4	46.2	1973	387	243.8	95.5	23.953	-161.634	-223.589	-223.589
24	2758.6	2776.6	30.5	823	172	244.9	95.9	6.795	-192.754	-252.41	-252.41
25	2894.9	2927.3	47	2444	484	245	95.6	37.045	-190.93	-250.72	-250.72
26	2941.9	2949.8	24.5	92	20	245	95.5	1.047	-281.784	-335.498	-335.498
27	3029.5	3044.3	29.9	649	138	250.1	97.1	5.182	-282.472	-335.498	-335.498
28	3158.6	3181.4	32	1345	267	250.4	96.2	13.887	-201.771	-260.76	-260.76
29	3190.6	3200	29.9	169	36	250.4	96.2	2.056	-187.226	-247.29	-247.29
30	3283.8	3298.9	30.9	654	138	250.3	96.4	5.217	-264.709	-319.047	-319.047
31	3325.8	3334.8	24.2	51	11	251.7	96.3	0.518	-228.1	-283.292	-283.292
32	3415.7	3427.2	21.7	280	65	244.6	94.4	2.091	-261.665	-316.228	-316.228
33	3476.9	3492	29.9	195	44	252.1	95.9	1.737	-162.355	-224.257	-224.257
34	3658.1	3669.6	24.2	127	30	248	95.6	0.932	-182.487	-242.901	-242.901
35	4994.7	4997.8	103.7	725	122	234.2	94.6	71.483	-197.057	-256.395	-256.395
36	5115.3	5117.2	62.5	720	121	234.8	94.5	42.782	-429.408	-471.575	-471.575
Triplicate 4											
1	18.4	20.5	22.6	711	119	235.6	95	13.938	-445.136	-486.14	-486.14
2	99.1	100.3	21.9	709	119	236.9	94.9	13.883	-442.59	-483.783	-483.783
3	198.3	199.8	22.2	708	119	237.1	94.7	13.931	-440.529	-481.874	-481.874
4	297.2	299.3	23.2	708	119	235.5	94.9	13.871	-443.538	-484.661	-484.661
5*	912.7	923.8	44.5	1688	438	245	96.8	11.02	0	-73.9	-73.9
6	1035.6	1040.8	20.3	74	19	248.8	98.1	0.684	-122.727	-187.557	-187.557
7	1056.3	1060.9	14.6	62	18	264.6	101.8	0.278	42.437	-34.599	-34.599
8	1163.9	1170.4	12.5	94	24	257.8	100.4	0.505	-139.596	-203.179	-203.179
9	1306.7	1313.4	24.5	225	55	252.3	98.2	1.478	-138.081	-201.777	-201.777
10	1331.1	1337	10	81	22	252.3	98.2	0.462	-76.794	-145.019	-145.019
11	1341.2	1343.9	15.3	51	13	252.3	98.2	0.411	-116.697	-181.973	-181.973
12	1360.2	1368.5	14.6	302	66	258.4	99.8	1.862	-234.912	-291.452	-291.452
13	1374.8	1379.6	19.9	177	37	258.4	99.8	1.405	-284.966	-337.807	-337.807
14	1455.3	1463.8	18.6	179	43	257.7	99.4	1.11	-165.248	-226.936	-226.936
15	1491.4	1501.5	39.1	618	120	262.8	100.7	4.679	-269.614	-323.59	-323.59
16	1611	1620.6	27.6	395	90	252.5	96	2.888	-187.603	-247.639	-247.639
17	1768.1	1779.2	31.5	454	103	251.3	97.6	3.277	-177.515	-238.297	-238.297
18	1926.6	1944.7	31.8	1406	269	250.2	97.4	12.643	-209.025	-267.478	-267.478
19	2016	2024.6	17.1	163	37	267.6	101.3	1.174	-241.313	-297.38	-297.38
20	2066.4	2075.6	15.9	93	21	263.1	100.6	0.655	-245.065	-300.855	-300.855
21	2082.3	2094.4	29.7	587	126	263.1	100.6	5.021	-210.504	-268.848	-268.848
22	2230.7	2254.5	39.1	1580	320	255.1	97.9	16.758	-205.845	-264.533	-264.533
23	2380.7	2394.3	29.5	539	121	258.4	98.5	4.676	-189.536	-249.429	-249.429
24	2524.3	2551.9	45.6	2161	429	256.5	98	28.31	-214.435	-272.488	-272.488
25	2664.3	2681.7	34.7	893	183	259.5	98.6	8.012	-212.299	-270.31	-270.31
26	2798.5	2833.4	47.7	2654	530	257.9	98.1	42.835	-221.987	-279.482	-279.482
27	2846.2	2854.7	24.9	101	22	257.9	98.1	1.244	-283.313	-336.276	-336.276
28	2933.5	2949.4	33	723	153	265.3	98.3	5.956	-209.094	-267.542	-267.542
29	3062.9	3086.7	32.2	1467	289	261.2	98.7	15.913	-211.224	-269.515	-269.515
30	3095.1	3104.3	31.6	187	39	261.2	98.7	2.216	-294.76	-346.878	-346.878
31	3186.2	3201.7	28.4	681	143	259	98.2	5.44	-249.894	-305.327	-305.327
32	3226.3	3236.2	26.8	57	13	257.8	97	0.556	-168.16	-229.633	-229.633
33	3315.8	3326.9	27.6	307	71	248.8	95.2	2.263	-181.138	-241.652	-241.652
34	3374.3	3390	32.4	209	46	255.7	97	1.86	-227.406	-284.501	-284.501
35	3554	3564.1	23.4	134	32	250.1	95.5	0.989	-180.991	-241.516	-241.516
36	4996.1	4997.6	101.8	662	111	237.1	94.9	65.242	-443.174	-484.323	-484.323
37	5115.9	5121.1	61.7	658	112	236.3	94.7	39.106	-442.881	-484.052	-484.052

1822

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Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs. VSMOW
Duplicate 1											
1	19.4	20.3	21.7	925	145	33.2	25.2	17.362	-447.44	-488.274	-488.274
2	99.1	99.9	21.7	923	145	33.3	25.6	17.34	-448.893	-489.62	-489.62
3	198.6	199.4	21.9	920	145	33.3	25.5	17.423	-448.652	-489.396	-489.396
4	298	298.9	21.7	907	144	33.4	25.7	17.284	-449.903	-490.555	-490.555
5	510	535	114.7	4790	1388	43.8	27.3	111.839	-23.421	-95.591	-95.591
6*	1140.3	1175.8	122.7	3283	845	55.4	31.6	788.29	0	-73.9	-73.9
7	1281.8	1305	86.6	87	20	51.8	30.5	2.786	-179.423	-240.064	-240.064
8	1419.5	1454.8	74.8	84	20	52.4	30.7	2.73	-180.743	-241.296	-241.296
9	1584	1616.2	86.1	162	37	50.8	30.2	6.351	-201.537	-260.544	-260.544
10	1674.3	1773.8	144.6	314	68	61.4	31.7	17.887	-258.692	-313.474	-313.474
11	1819.8	1848.8	86.8	81	13	82.2	36.7	1.508	-313.224	-363.977	-363.977
12	1910.5	1951.9	113.5	648	145	58.8	31.7	27.744	-220.743	-278.33	-278.33
13	2073.5	2119.1	137.5	447	102	49.3	29.6	25.276	-216.022	-273.958	-273.958
14	2233	2326.2	171.4	5244	1228	51.4	29.8	278.626	-226.011	-283.209	-283.209
15	2405.2	2448.9	118.5	929	209	66.2	33.6	42.733	-224.787	-282.075	-282.075
16	2549.6	2646.8	164.1	5384	1266	58.7	30.9	295.353	-222.429	-279.892	-279.892
17	2713.7	2755.9	122.1	1018	230	58.7	30.9	49.748	-215.116	-273.119	-273.119
18	2846.4	2962.4	166.6	6688	1610	75.3	34.7	426.653	-222.666	-280.111	-280.111
19	3012.9	3056	119.8	2176	484	75.3	34.7	79.643	-222.573	-280.025	-280.025
20	3131	3247.2	182.8	6795	1620	83.2	36.7	444.683	-230.884	-287.722	-287.722
21	3283.8	3328.5	102.8	2317	506	83.2	36.7	75.729	-224.946	-282.222	-282.222
22	3397.3	3465.2	111.6	3382	764	99.9	40.3	146.283	-226.919	-284.05	-284.05
23	3509.3	3529.8	35.3	323	63	325.5	92.5	4.913	-322.519	-372.585	-372.585
24	3544.6	3624.5	96.6	1716	349	325.5	92.5	57.701	-288.687	-341.253	-341.253
25	3641.2	3645.6	75	607	128	325.5	92.5	16.785	-257.307	-312.192	-312.192
26	3739.6	3788.5	105.1	528	111	122.8	45.4	17.996	-249.109	-304.6	-304.6
27	3848.3	3886.4	81.5	299	67	83.6	36.6	10.154	-209.226	-267.665	-267.665
28*	3960.3	4029.9	122.9	2994	701	128.9	46.7	123.668	0	-244.1	-244.1
29	4996.4	4997.2	101.4	859	133	41.8	28.1	80.745	-318.064	-484.525	-484.525
30	5115.7	5116.7	61.9	842	134	33.5	25.9	48.833	-313.851	-481.34	-481.34
Duplicate 2											
1	19.4	20.3	21.7	852	133	33.5	26	16.015	-451.048	-491.615	-491.615
2	99.1	99.9	21.7	850	133	33.6	25.7	15.992	-450.04	-490.682	-490.682
3	198.6	199.4	21.9	835	133	33.6	25.8	16.069	-451.068	-491.634	-491.634
4	298	299.1	21.9	837	132	33.5	25.6	15.943	-450.576	-491.178	-491.178
5	510	536.1	116.8	5328	1552	44.8	28.7	127.017	-28.951	-100.712	-100.712
6*	1140.5	1176.5	123.7	3573	1039	57.2	32.1	97.967	0	-73.9	-73.9
7	1281.4	1304.8	89.2	88	20	53.3	31	2.909	-187.986	-247.994	-247.994
8	1418.7	1454.4	77.5	83	20	53.6	31	2.83	-185.794	-245.964	-245.964
9	1583.2	1615.6	87.6	157	37	51.7	29.7	6.472	-174.745	-235.732	-235.732
10	1674.3	1774	144.8	303	65	62.8	32.7	18.009	-263.133	-336.11	-336.11
11	1820	1848	88.2	53	11	87.1	37.5	1.201	-288.991	-341.535	-341.535
12	1909.8	1950.6	114.5	617	138	59.6	32	27.645	-224.448	-281.759	-281.759
13	2072.9	2118	139.8	428	98	49.7	29.5	25.035	-214.886	-272.887	-272.887
14	2232.5	2324.9	170.8	5178	1210	51.7	29.8	274.568	-226.504	-283.665	-283.665
15	2404.1	2447.8	116.5	897	201	65.7	33.4	41.863	-225.698	-282.917	-282.917
16	2549	2644.7	163.4	5284	1241	58.6	31	286.939	-222.912	-280.339	-280.339
17	2712.8	2753.8	122.3	983	221	89.2	38.8	44.328	-225.876	-283.083	-283.083
18	2845.7	2959.4	165.3	6542	1569	74.5	34	410.254	-222.121	-279.607	-279.607
19	3011.1	3054.1	117.5	2183	481	74.5	34	78.177	-220.51	-278.115	-278.115
20	3129.8	3243.3	181.1	6580	1563	81.8	36.4	422.311	-231.093	-287.915	-287.915
21	3290.9	3325.2	103.7	2205	481	81.8	36.4	70.93	-225.161	-282.422	-282.422
22	3395.6	3461.2	109.7	3231	727	96.6	39.3	136.412	-226.44	-283.606	-283.606
23	3505.3	3526.5	37.6	524	109	96.6	39.3	12.571	-245.362	-301.13	-301.13
24	3543	3620.7	94.9	1861	384	96.6	39.3	74.344	-266.285	-320.506	-320.506
25	3637.9	3684	71.9	807	181	96.6	39.3	31.101	-224.616	-282.102	-282.102
26	3745.7	3782.5	94.7	541	114	123.8	45.4	16.448	-246.855	-302.513	-302.513
27	3845.4	3881.1	76.7	310	69	81	35.8	9.452	-207.935	-266.469	-266.469
28*	3958.7	4029.7	129.2	2864	672	121.8	45	124.213	0	-244.1	-244.1
29	4996.4	4997.2	101.4	792	123	42.8	28.2	74.303	-320.218	-486.153	-486.153
30	5115.7	5116.7	61.9	784	123	33.5	25.7	45.025	-315.322	-482.452	-482.452

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Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (pemitil vs. C16)	dT (pemitil vs. C16)	dD (pemitil vs. VSMOW)
Duplicate 1											
1	19.4	20.5	21.5	86	16	32.9	25.4	1.664	-370.206	-416.748	-416.748
2	99.1	100.1	21.5	85	17	32.9	25.4	1.654	-362.963	-410.04	-410.04
3	198.6	199.6	21.7	85	17	32.9	24.9	1.653	-346.373	-394.676	-394.676
4	298	299.1	21.7	84	18	33.7	23.7	1.631	-289.573	-342.074	-342.074
5	505.8	531.7	112.4	4802	1399	40.9	27.5	110.722	-30.696	-102.327	-102.327
6	781.5	794.4	64	274	66	37.6	26.7	5.211	-146.888	-209.933	-209.933
7	1142.8	1175.4	111	2951	851	38.3	26.9	73.266	0	-73.9	-73.9
8	1682	1703.1	59.6	178	35	51.6	29.5	4.486	-312.652	-363.447	-363.447
9	1758.3	1773.4	53.1	96	19	99.5	39.9	0.638	-366.548	-413.453	-413.453
10	1823.7	1840.5	50.6	170	35	51.5	29.6	3.066	-281.045	-334.175	-334.175
11	1918.6	1933	33.6	138	31	44.2	28.1	2.264	-210.189	-268.556	-268.556
12	2082.7	2097.1	50.4	135	31	46.2	28.7	2.394	-180.908	-241.438	-241.438
13	2242.4	2258.3	83.8	632	138	40.5	26.5	14.269	-196.868	-255.293	-255.293
14	2390.1	2419.2	76.7	248	55	45.3	28.4	4.915	-196.671	-256.037	-256.037
15	2553.4	2583.4	62.3	803	175	41.3	27.2	18.527	-208.925	-267.386	-267.386
16	2704.5	2721.8	70.2	211	47	47.4	28.5	4.196	-182.164	-242.602	-242.602
17	2847.2	2876.7	56.6	741	163	44.1	28	16.575	-200.544	-259.624	-259.624
18	2903.8	2909.1	48.5	107	25	44.1	28	2.944	-206.787	-265.406	-265.406
19	2990.4	3009	65.4	266	60	52.8	29.9	5.26	-188.945	-248.882	-248.882
20	3124.3	3162.2	58.7	1105	246	46.3	28.4	27.333	-197.234	-256.558	-256.558
21	3183.1	3190	76.9	339	76	46.3	28.4	13.805	-227.859	-284.92	-284.92
22	3260.8	3277.7	44.3	227	51	67.2	33.4	4.11	-205.428	-264.147	-264.147
23	3376.2	3418.4	62.3	740	164	60.2	31.3	17.98	-203.779	-262.62	-262.62
24	3438.5	3445.2	29.5	236	54	60.2	31.3	4.623	-203.742	-262.585	-262.585
25	3469	3494.9	52.5	207	42	133.5	48.8	3.711	-299.061	-350.86	-350.86
26	3521.4	3532.9	32.2	52	11	133.5	48.8	-0.06	-275.261	-328.819	-328.819
27	3554.3	3584.6	55.4	274	116	91.3	39.4	13.092	-273.167	-326.88	-326.88
28	3632.8	3650.2	36.8	590	57	122.5	45.6	4.068	-187.936	-247.947	-247.947
29	3742.8	3751.3	66.7	308	67	83.7	37	6.369	-169.758	-214.64	-214.64
30	3842	3873.4	48.1	71	17	62	32.4	1.543	-169.996	-231.333	-231.333
31*	3866.8	4037.9	127.1	2955	686	77.2	36	123.052	0	-244.1	-244.1
32	4995.7	4996.8	101.2	58	11	42.8	28.5	4.94	-238.571	-424.572	-424.572
33	5115.3	5123.4	61.4	59	13	32.7	25.3	3.486	-146.695	-354.967	-354.967
Duplicate 2											
1	19.4	20.5	21.5	57	13	32.9	25.1	1.121	-296.288	-348.292	-348.292
2	99.1	102.4	21.5	57	13	32.9	25.3	1.116	-304.645	-356.032	-356.032
3	198.6	200.8	21.7	56	12	32.9	25.4	1.115	-322.753	-372.803	-372.803
4	298	299.1	21.5	56	12	32.9	25.3	1.099	-315.258	-365.86	-365.86
5	504.7	533.4	118.1	6106	1807	43	28.4	147.264	-32.103	-103.631	-103.631
6	780.8	794.4	67.7	351	86	38.3	26.8	1.719	-139.577	-203.162	-203.162
7	1143.2	1178.1	114.5	3599	391	27.2	22.2	92.177	0	-73.9	-73.9
8	1681	1701.9	59.6	159	31	50.1	37	3.22	-322.934	-372.569	-372.569
9	1757.1	1772.1	53.1	87	19	92	37.7	0.608	-138.176	-201.864	-201.864
10	1822.9	1839.2	50.2	150	31	49.8	29.2	2.747	-271.205	-325.063	-325.063
11	1917.6	1931.8	33.9	124	28	43.3	27.6	2.047	-182.441	-242.858	-242.858
12	2081.4	2096.9	50.4	28	28	45.2	28.5	2.154	-173.183	-234.285	-234.285
13	2241.3	2266.2	73.6	125	42	47.5	27	12.661	-204.259	-263.065	-263.065
14	2389.1	2417.5	75.2	223	50	45.3	28.1	4.397	-182.323	-242.749	-242.749
15	2552.3	2581.1	61.4	734	161	41.3	27.5	16.522	-209.447	-267.869	-267.869
16	2703.2	2720.3	68.6	187	42	46.9	28.6	3.772	-184.107	-244.402	-244.402
17	2846.2	2874.4	55.8	873	149	44.2	27.5	14.744	-191.797	-251.523	-251.523
18	2902	2907.8	48.3	53	23	44.3	27.5	2.613	-195.956	-272.592	-272.592
19	2989.1	3007.1	64.8	238	54	52	30	4.686	-197.499	-256.804	-256.804
20	3123.1	3159	57.3	1011	226	46.1	28.1	24.344	-192.689	-252.35	-252.35
21	3180.4	3187.3	78	298	67	46.1	28.1	12.388	-219.545	-277.22	-277.22
22	3259.1	3275.7	44.1	201	45	64.7	33	3.669	-201.252	-260.279	-260.279
23	3374.3	3415.3	61.4	675	150	58.7	31.1	16.061	-232.124	-281.067	-281.067
24	3435.8	3442.6	30.1	208	47	58.7	31.1	4.158	-199.073	-258.261	-258.261
25	3466.7	3492.2	52	188	39	122.9	46.2	3.417	-284.032	-336.942	-336.942
26	3519.1	3530.2	32	77	17	93.7	39.5	0.922	-183.185	-243.548	-243.548
27	3551.7	3581.2	55.2	525	106	85.6	38.1	11.856	-271.04	-324.91	-324.91
28	3606.9	3615.1	21.9	65	23	65.1	37	1.605	-377.636	-321.204	-321.204
29	3630.3	3647.9	37.2	252	56	85.6	38.1	4.692	-209.851	-268.243	-268.243
30	3739.8	3762.8	68.1	320	70	79.4	36.1	6.547	-210.339	-268.695	-268.695
31	3841	3871.9	47.9	67	17	61.1	31.8	1.454	-109.096	-174.934	-174.934
32*	3964.9	4044.6	150.5	3422	801	75.8	36	155.829	0	-244.1	-244.1
33	4995.7	4996.8	101.8	1519	427	42.7	28.7	145.015	-288.454	-462.15	-462.15
34	5115.3	5116.1	62.1	1527	252	33	25.5	86.71	-285.116	-459.619	-459.619
NEW											
TriPLICATE 1											
1	18.8	20.7	22.4	589	99	239.7	94.9	11.529	-439.002	-480.46	-480.46
2	99.1	100.3	21.7	587	99	239.1	95.2	11.511	-441.374	-482.657	-482.657
3	197.9	201.7	22.6	587	98	238.4	95.2	11.569	-442.079	-483.31	-483.31
4	298	306.8	22.2	586	98	238.5	95.5	11.469	-444.331	-485.395	-485.395
5	370.1	386.6	39.1	170	49	237.2	94.8	4.321	-41.132	-111.993	-111.993
6*	904.6	929	56.2	8420	2317	245.7	86	99.614	0	-73.9	-73.9
7	1026.8	1036.2	20.3	56	15	264.8	102	0.658	-144.548	-207.766	-207.766
8	1047.1	1052.7	23	85	24	264.8	102	0.768	-72.672	-141.201	-141.201
9	1105.2	1116.3	25.1	60	15	276.7	106.2	0.954	-205.765	-264.459	-264.459
10	1155.1	1163.7	28.4	133	35	310.3	113.8	1.685	-193.404	-253.012	-253.012
11	1299.1	1310.2	41.0	210	51	312.4	113.7	5.91	-234.522	-291.187	-291.187
12	1326.5	1333.6	25.3	246	67	312.4	113.7	2.785	-162.626	-224.508	-224.508
13	1351.8	1366.4	44.1	1043	209	312.4	113.7	19.26	-326.493	-376.265	-376.265
14	1407.8	1419.5	20.9	385	85	309.1	111.4	4.649	-255.663	-310.669	-310.669
15	1426.7	1439.8	22.2	886	175	309.1	111.4	9.264	-313.204	-363.032	-363.032
16	1450.9	1465.4	23.8	395	60	309.1	111.4	3.545	-287.52	-367.52	-367.52
17	1475.1	1500.6	48.9	1500	278	307.2	109.9	14.713	-270.769	-324.66	-324.66
18	1561.9	1571.9	27.4	164	42	296.5	109.2	1.54	-168.36	-229.818	-229.818
19	1601.6	1618.1	30.5	1076	241	282.6	106.8	12.048	-199.361	-258.926	-258.926
20	1632.1	1639.8	24.2	158	44	282.6	106.8	1.714	-114.339	-179.79	-179.79
21	1713	1727	35.3	299	79	287.9	107	3.995	-102.384	-168.718	-168.718
22	1759.4	1775.7	38.5	953	225	286.6	106.9	11.995	-181.702	-242.174	-242.174
23	1809.3	1820	25.9	53	14	285.3	106.7	0.735	-151.447	-214.155	-214.155
24	1915.1	1952.7	44.3	3729	769	273.6	103.4	63.86	-214.802	-272.926	-272.926
25	1959.4	1985.5	18.8	210	51	273.6	103.4	2.025	-220.958	-287.79	-287.79
26	1978.2	1992.4	24.9	93	21	273.6	103.4	1.741	-239.423	-295.629	-295.629
27	2018.7	2037.3	35.1	64	16	292.4	107.2	1.028	-125.554	-190.175	-190.175
28	2073.3	2095.4	53.3	1556	338	323.8	115.6	21.235	-206.188	-264.851	-264.851
29	2169.8	2180.9	40.3	74	19	288.5	106.6	1.355	-132.561	-196.655	-196.655
30	2223.5	2266.8	60	3965	793	303.7	103.7	63.93	-213	-262.641	-262.641
31	2283.5	2293.4	26.8	64	328.9	314.8	114.8	3.414	-190.084	-249.937	-249.937
32	2335.2	2346.7	26.8	73	19	332.1	116.5	0.813	-118.915	-184.027	-184.027
33	2365.5	2394.5	55.8	1171	277	322.5	113.5	18.246	-		

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57	3489.9	3508.1	33.2	275	62	335.4	115.7	2.668	-223.025	-280.443	-280.443
58	3533.6	3545.3	19	102	25	311.4	109.4	0.937	-146.338	-209.423	-209.423
59	3556.2	3566.2	27.8	672	153	311.4	109.4	5.881	-171.191	-232.44	-232.44
60	3580.4	3597.3	27.2	670	145	311.4	109.4	6.932	-205.015	-263.764	-263.764
61	3607.5	3621.8	29.7	383	69	311.4	109.4	6.575	-210.528	-268.87	-268.87
62	3637.2	3646.8	18.4	200	46	311.4	109.4	2.524	-227.777	-280.214	-280.214
63	3655.6	3657.5	9.6	62	15	311.4	109.4	0.447	-218.012	-275.801	-275.801
64	3665.2	3674.8	23.4	36	31	311.4	109.4	1.287	-176.432	-237.294	-237.294
65	3776.6	3784.6	23.6	121	31	299.1	107.1	0.751	-172.752	-233.886	-233.886
66	3800.2	3814.9	25.1	255	60	299.1	107.1	2.344	-191.843	-251.566	-251.566
67	3825.3	3841.2	24.9	226	53	299.1	107.1	3.088	-203.005	-261.903	-261.903
68	3850.2	3864.6	23	115	27	299.1	107.1	1.819	-232.272	-289.007	-289.007
69	3990.2	3997.5	21.5	80	21	294.8	105.9	0.524	-121.118	-186.067	-186.067
70	4011.8	4030.1	27	390	94	294.8	105.9	3.702	-160.829	-222.844	-222.844
71	4038.7	4054.2	23.8	419	98	294.8	105.9	4.595	-191.386	-251.142	-251.142
72	4052.5	4072.2	18.6	117	28	294.8	105.9	1.565	-232.959	-289.644	-289.644
73	4229.7	4250.6	31.1	398	95	279.2	102.1	5.16	-156.569	-218.899	-218.899
74	4260.9	4279.5	28.4	404	93	279.2	102.1	5.792	-193.981	-253.546	-253.546
75	4289.3	4301.2	27.6	100	23	279.2	102.1	1.978	-238.058	-294.365	-294.365
76	4510.6	4540.7	44.5	233	57	267.8	99.5	4.303	-163.398	-225.223	-225.223
77	4555.2	4585.3	43.9	454	103	267.8	99.5	9.71	-197.571	-256.871	-256.871
78	4599	4609.5	31.8	102	23	267.8	99.5	2.291	-259.432	-314.16	-314.16
79	4912.3	4935.7	44.9	68	17	265.6	99	1.68	-144.855	-208.05	-208.05
80	4957.3	4978	24.5	136	36	265.6	99	0.89	-19.862	-55.506	-55.506
81	4993.2	5009	102.2	1899	1899	237.2	95.8	185.624	-426.715	-469.061	-469.061
82	5112.3	5113.8	62.5	1887	330	239.4	95.8	111.158	-426.493	-468.875	-468.875

Triplicate 2

1	19.4	20.5	23.8	1865	325	239.8	95.6	36.236	-427.019	-469.362	-469.362
2	99.1	100.1	22.6	1862	326	237.1	95.1	36.227	-426.945	-469.293	-469.293
3	198.8	199.8	22.4	1863	325	237.3	95.2	36.331	-427.473	-469.782	-469.782
4	296.6	299.3	24.5	1853	324	238.4	95.4	36.068	-427.092	-469.43	-469.43
5	367.8	379.1	47.2	224	66	236.8	93.4	5.587	5.622	-68.693	-68.693
6	671.1	675.8	15.3	53	15	246.5	97.6	0.256	-12.886	-85.833	-85.833
7	906.4	929.4	54.5	7887	2128	246.6	97.6	88.628	0	-73.9	-73.9
8	1024.9	1032.7	22.8	87	24	246.9	103.1	0.718	-127.643	-192.11	-192.11
9	1047.7	1052.7	15.5	142	41	266.9	103.1	0.713	-39.539	-110.517	-110.517
10	1106.4	1117.1	20.7	100	24	276.8	106	0.68	-231.751	-288.524	-288.524
11	1155.6	1164.3	27.6	156	301	308	113.8	1.626	-200.148	-259.257	-259.257
12	1300.4	1310.6	27.4	383	97	316.8	115.4	6.269	-238.814	-296.158	-296.158
13	1327.8	1335.3	25.3	260	64	316.4	115.4	3.068	-199.914	-231.257	-231.257
14	1353.1	1365.2	44.9	1015	208	316.4	115.4	20.608	-331.461	-380.866	-380.866
15	1408.7	1420.6	21.1	383	84	314.5	113.4	4.731	-257.628	-312.489	-312.489
16	1429.8	1438.8	22.8	884	176	314.5	113.4	10.098	-315.194	-385.801	-385.801
17	1452.6	1463.6	24	396	93	314.4	113.4	3.914	-214.521	-272.568	-272.568
18	1476.6	1501.7	54.4	1523	290	314.5	113.4	15.738	-285.652	-338.442	-338.442
19	1562.3	1572.3	29.3	168	43	300.7	111.3	1.732	-180.073	-240.666	-240.666
20	1602.8	1618.3	30.7	1142	255	289.7	107.8	13.072	-198.357	-257.598	-257.598
21	1633.5	1640.7	27.2	477	48	289.7	107.8	1.942	-97.438	-164.138	-164.138
22	1715.3	1727.2	34.5	323	43	294.9	110.3	4.322	-118.957	-184.066	-184.066
23	1760	1777.1	49.3	1052	244	295.1	108.8	13.084	-176.292	-237.164	-237.164
24	1810.4	1820.6	30.9	58	15	291	108	0.845	-160.599	-222.63	-222.63
25	1916.1	1955	45.1	3849	596	276.5	104.8	68.503	-215.661	-273.623	-273.623
26	1961.3	1963.1	16.5	246	59	276.5	104.8	2.136	-226.974	-283.175	-283.175
27	2030.4	2038.8	38.2	70	17	287.9	113.6	1.136	-145.771	-208.899	-208.899
28	2074.5	2097.3	49.1	1616	361	331.8	118	22.877	-203.307	-262.183	-262.183
29	2170	2183.6	38.2	81	22	292.7	108	1.528	-94.822	-161.714	-161.714
30	2224.2	2269.9	60.6	3787	636	290.4	105.6	87.264	-205.277	-264.007	-264.007
31	2284.8	2294.8	26.3	382	20	280.4	105.6	5.316	-215.849	-273.798	-273.798
32	2311.1	2324.4	12.7	91	31	280.4	105.6	0.824	-236.859	-293.043	-293.043
33	2323.9	2347.5	40.1	151	38	280.4	105.6	3.296	-173.968	-235.012	-235.012
34	2369.9	2398.9	52.7	1352	298	327.7	116.4	13.989	-191.486	-251.235	-251.235
35	2450.7	2476.2	63.1	151	34	317.6	113.8	4.017	-234.264	-290.852	-290.852
36	2515.9	2552.8	78.7	2884	788	295.4	113.8	81.044	-285.133	-354.813	-354.813
37	2573.6	2605.5	40.8	538	125	292.2	107.4	9.733	-211.975	-270.21	-270.21
38	2614.4	2636.3	46.4	223	55	292.2	107.4	5.627	-177.312	-238.109	-238.109
39	2660.8	2688.2	50.6	1438	332	292.2	107.4	28.394	-192.399	-252.081	-252.081
40	2711.4	2771.1	84.9	166	40	292.2	107.4	6.699	-188.916	-248.855	-248.855
41	2798.3	2843.4	81.9	4985	1230	312.8	112	160.549	-200.082	-259.196	-259.196
42	2860.2	2899.2	32.2	179	15	312.8	112	22.417	-112.767	-292.72	-292.72
43	2905.5	2916.6	28.8	1789	24	447.4	145.2	0.482	-354.735	-402.42	-402.42
44	2936.4	2962.2	47	1364	309	379.7	128.5	24.729	-193.917	-253.487	-253.487
45	2983.5	2994.3	21.1	63	14	379.7	128.5	0.74	-233.392	-290.044	-290.044
46	3004.6	3028.8	43.3	465	96	379.7	128.5	9.908	-288.693	-322.737	-322.737
47	3047.8	3120.8	78.4	305	34	379.7	128.5	111.613	-199.528	-286.775	-286.775
48	3126.2	3134	32.2	1900	419	379.7	128.5	32.531	-279.83	-333.06	-333.06
49	3158.4	3167	17.3	228	51	379.7	128.5	2.58	-256.425	-311.375	-311.375
50	3175.8	3176.2	9.6	87	19	379.7	128.5	0.558	-255.033	-310.086	-310.086
51	3185.4	3228.8	69	3237	721	379.7	128.5	94.338	-251.183	-306.521	-306.521
52	3254.3	3271.1	23.4	1061	212	379.7	128.5	11.95	-273.928	-327.585	-327.585
53	3277.7	3283.8	26.8	147	33	379.7	128.5	1.381	-332.77	-382.078	-382.078
54	3323.1	3354.9	40.3	2422	503	337.6	118.6	36.189	-196.508	-255.886	-255.886
55	3363.4	3376.8	24.5	1020	222	337.6	118.6	11.287	-231.353	-288.156	-288.156
56	3387.9	3421.7	43.1	1793	359	337.6	118.6	36.287	-247.14	-302.776	-302.776
57	3430.6	3452.2	10.7	305	10	343.2	118.6	0.805	-337.198	-361.146	-361.146
58	3441.6	3453.5	21.9	1384	26	337.6	118.6	4.035	-211.962	-270.198	-270.198
59	3469.6	3481.9	25.1	88	21	349.1	120.4	1.066	-176.411	-237.274	-237.274
60	3494.7	3513.7	33.4	299	66	349.1	120.4	3.032	-227.195	-284.305	-284.305
61	3538.8	3550.1	18.4	108	26	321.1	113.9	1.065	-221.113	-278.672	-278.672
62	3557.2	3571.2	26.8	305	32	312.1	113.9	7.004	-186.382	-246.508	-246.508
63	3585	3602.1	27.8	200	48	312.4	110.8	8.1	-204.198	-263.008	-263.008
64	3612.8	3628.2	29.9	453	103	312.4	110.8	7.884	-206.336	-264.988	-264.988
65	3642.7	3651.2	17.6	241	56	312.4	110.8	2.947	-220.309	-277.928	-277.928
66	3680.2	3691.9	9	80	19	312.4	110.8	0.578	-189.362	-249.062	-249.062
67	3699.2	3680.1	23.2	200	48	312.4	110.8	1.931	-162.753	-224.625	-224.625
68	3692.8	3707.2	26.5	62	15	313.5	111.8	0.732	-196.276	-255.672	-255.672
69	3721.5	3732.9	22.6	59	15	306.7	109.8	0.619	-167.649	-229.159	-229.159
70	3780.2	3789.2	23.2	148	38	306.6	109.8	1.014	-113.658	-179.158	-179.158
71	3803.4	3819.1	26.1	298	71	306.6	109.8	2.867	-167.264	-228.803	-228.803
72	3830.6	3845.8	24.7	247	50	338.9	117.1	3.086	-177.119	-237.93	-237.93
73	3855.2	3869.2	23	111	25	338.9	117.1	1.497	-211.265	-269.553	-269.553</

1922 CONT

13	1599.9	1607.4	19.2	184	45	245.3	97.9	1.041	-143.138	-206.46	-206.46
14	1712.5	1718.6	16.5	53	14	244.4	98.1	0.336	-85.183	-152.788	-152.788
15	1755.4	1765.2	21.9	173	43	244.4	98.1	1.079	-163.315	-225.146	-225.146
16	1913.6	1927.4	27.4	808	169	243.7	97.6	5.823	-193.322	-252.936	-252.936
17	2067.8	2078.7	22.8	315	73	249.7	99.6	2.026	-193.428	-253.034	-253.034
18	2219.4	2236.5	30.7	980	197	248.6	98.4	8.002	-193.189	-252.822	-252.822
19	2367.3	2378.2	22.6	256	62	257	100.1	1.71	-157.556	-219.812	-219.812
20	2509.9	2528.1	35.5	902	191	256	99.8	7.694	-189.66	-249.544	-249.544
21	2557.5	2565.5	17.8	52	12	265.7	102.1	0.497	-201.072	-260.113	-260.113
22	2650.1	2662.7	24.7	331	79	262.2	101	2.362	-164.356	-226.11	-226.11
23	2797.2	2807.5	34.3	1569	319	265.5	101.6	14.611	-203.213	-262.095	-262.095
24	2829.7	2840.9	27.6	204	47	278.7	103.4	1.537	-187.317	-247.375	-247.375
25	2921.4	2933.1	24	289	66	263.7	101.4	2.181	-192.419	-252.1	-252.1
26	2986.4	2997.5	20.3	86	20	263.1	101	0.643	-185.834	-246.001	-246.001
27	3047.6	3070	31.6	875	186	263.6	101.4	7.95	-188.382	-248.361	-248.361
28	3079.2	3091.7	17.6	343	71	263.6	101.4	2.918	-253.386	-317.821	-317.821
29	3096.8	3099.7	14.8	156	35	263.6	101.4	1.163	-277.972	-331.33	-331.33
30	3173.5	3191.6	32.6	801	166	268.7	102.3	7.351	-249.552	-305.01	-305.01
31	3213	3224.5	28	110	25	266.9	101	0.973	-246.524	-302.206	-302.206
32	3303.9	3317.2	25.1	379	89	258.9	99.9	2.844	-179.765	-240.381	-240.381
33	3338.4	3348.2	23.8	91	22	260	99.7	0.866	-197.981	-257.25	-257.25
34	3383.4	3380.4	31.1	290	64	269.5	101.8	2.508	-207.055	-265.654	-265.654
35	3545.5	3553.8	18.6	62	16	260.6	99.8	0.438	-191.242	-251.01	-251.01
36	3572.9	3585	23.4	68	17	252.8	97.8	0.616	-161.886	-223.822	-223.822
37	4192.3	4226.1	89	211	50	271.5	102.8	9.237	-201.385	-260.403	-260.403
38	4986.1	4997.6	103.5	1581	274	234.6	96.4	155.195	-431.418	-473.436	-473.436
39	5114.6	5117.2	64.2	1571	272	238.8	97	92.693	-430.844	-472.904	-472.904

2022

(not abundant enough)

Peak	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs. VSMOW
Duplicate 1											
1	19.4	20.5	21.9	1134	183	33.6	25.8	21.721	-449.556	-490.234	-490.234
2	99.1	99.9	21.9	1131	183	33.6	25.4	21.694	-448.051	-488.84	-488.84
3	198.6	199.6	21.9	1136	182	33.6	25.4	21.775	-448.449	-489.209	-489.209
4	298	299.1	21.9	1142	182	33.7	25.7	21.62	-449.081	-489.794	-489.794
5	509.3	532.3	108.5	3777	1082	42.7	28.1	84.673	-33.92	-105.313	-105.313
6*	1138.8	1169.6	107.4	2648	763	41.4	27.4	65.155	0	-73.9	-73.9
7	1584.2	1600.3	59.1	126	30	45.2	28.4	2.484	-143.247	-206.561	-206.561
8	1738.9	1764.2	52	56	14	50	29.3	1.113	-99.689	-166.222	-166.222
9	1811.2	1836.6	62.9	401	79	50	29.3	8.48	-298.341	-340.932	-340.932
10	1911.9	1927.6	57.5	128	31	46.5	28.5	2.406	-145.362	-208.52	-208.52
11	2022.9	2043.8	51.8	73	19	44.2	28	1.421	-82.811	-150.591	-150.591
12	2076.8	2090.8	52	80	20	49.7	29.3	1.422	-93.5	-160.49	-160.49
13	2233.4	2256.8	68.8	313	71	42.1	27.4	6.567	-174.85	-235.829	-235.829
14	2393.7	2411.2	79.4	134	32	45.2	28.2	4.733	-182.475	-242.89	-242.89
15	2542.9	2568.8	77.7	366	82	42.5	27.5	7.918	-180.789	-241.329	-241.329
16	2693.6	2713.9	61.4	174	40	43.5	27.9	3.526	-169.277	-230.668	-230.668
17	2835.7	2864.3	94.1	465	104	43.7	27.7	10.927	-188.316	-248.299	-248.299
18	2977.2	2999.1	70.6	207	48	49.9	29	4.203	-158.933	-221.088	-221.088
19	3111	3139.4	75	443	99	45.3	28	10.224	-184.791	-245.035	-245.035
20	3246.2	3264.4	50.6	113	27	49.7	28.8	2.191	-147.947	-210.914	-210.914
21	3367.8	3398.5	83	429	98	45	27.7	10.191	-166.572	-228.163	-228.163
22	3615.1	3640.2	70.4	336	78	53.6	29.9	7.296	-152.146	-214.803	-214.803
23	3728.4	3751.6	65.6	126	30	55.3	29.9	2.676	-141.159	-204.628	-204.628
24	3840	3864.8	47.4	63	16	51.8	29.5	1.389	-116.282	-181.588	-181.588
25*	3949.1	4018.4	131.7	2424	558	61.3	31.5	98.757	0	-244.1	-244.1
26	4995.5	4996.6	101.6	1070	168	40	27.5	101.114	-312.81	-480.553	-480.553
27	5115.1	5116.1	61.9	1050	169	33.5	25.6	60.945	-309.951	-478.392	-478.392
Duplicate 2											
1	19.4	20.3	21.7	1064	168	33.5	25.5	19.986	-448.448	-489.207	-489.207
2	99.1	99.9	21.7	1063	167	33.5	25.4	19.96	-447.846	-488.65	-488.65
3	198.6	199.4	21.9	1044	168	33.5	25.4	20.055	-447.462	-488.294	-488.294
4	298	299.1	21.9	1046	167	33.6	25.5	19.897	-447.587	-488.41	-488.41
5	509.1	533	110.4	4116	1182	43.2	28.5	93.435	-31.556	-103.124	-103.124
6*	1139.9	1172.1	109.9	2957	850	41.7	28	74.037	0	-73.9	-73.9
7	1585.3	1600.3	58.9	131	32	45.2	28.4	2.535	-142.829	-206.174	-206.174
8	1738.7	1764.2	52.5	59	15	49.9	29.2	1.143	-89.584	-156.864	-156.864
9	1812.9	1838.8	60.8	415	81	49.9	29.3	8.572	-291.117	-343.504	-343.504
10	1913	1927.6	56.8	133	32	46.1	28	2.475	-115.348	-180.724	-180.724
11	2022.9	2043.6	53.1	75	19	44.2	27.9	1.447	-76.655	-144.89	-144.89
12	2077.7	2090.6	50.8	84	21	49	29.6	1.494	-157.078	-219.37	-219.37
13	2234.8	2257	67.7	325	73	42	27.4	6.66	-176.902	-237.729	-237.729
14	2394.9	2411	77.5	139	33	45	28.4	4.81	-198.809	-258.017	-258.017
15	2544.6	2569	76.5	378	85	42.4	27.5	8.021	-181.069	-241.588	-241.588
16	2694.6	2713.7	59.6	180	42	43.4	28	3.567	-177.204	-238.009	-238.009
17	2837.2	2864.3	92.6	480	107	43.5	27.3	11.025	-175.084	-236.046	-236.046
18	2979.1	2998.9	69.4	214	49	49.7	29.1	4.231	-171.301	-232.542	-232.542
19	3112.6	3139.6	73.2	456	102	45	28	10.263	-183.412	-243.758	-243.758
20	3247.4	3264.2	49.1	116	27	49	28.5	2.228	-139.97	-203.526	-203.526
21	3368.2	3398.5	83.6	442	101	44.8	27.3	10.248	-156.332	-218.679	-218.679
22	3616.7	3639.9	68.3	346	80	52	29.5	7.377	-148.427	-211.359	-211.359
23	3730.2	3751.1	63.5	141	32	54.5	30	2.914	-164.289	-226.048	-226.048
24	3840.4	3864	46.4	66	17	51.5	29.3	1.402	-107.656	-173.6	-173.6
25*	3951.4	4024.3	135	2664	613	58.6	31	109.87	0	-244.1	-244.1
26	4995.5	4996.6	101.6	983	154	39.6	27.8	93.09	-315.65	-482.7	-482.7
27	5115.1	5115.9	61.9	969	155	33.4	25.6	58.17	-310.684	-478.946	-478.946

2222

Peak	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs. V8MOW
Duplicate 1											
1	19.4	20.3	22.4	1802	300	33	26.6	34.589	-435.268	-477.002	-477.002
2	99.1	100.1	22.4	1806	300	33.1	26.1	34.485	-434.383	-476.182	-476.182
3	198.6	199.6	22.6	1806	299	33.1	26.3	34.673	-434.469	-476.262	-476.262
4	298	299.1	22.4	1816	298	33.1	26.6	34.379	-435.234	-476.97	-476.97
5	508.3	528.6	99.3	2248	633	37.8	27.8	49.354	-24.037	-96.161	-96.161
6*	1141.8	1185.9	132.9	5583	1668	85.3	35.2	171.048	0	-73.9	-73.9
7	1262.6	1302.5	64.6	164	37	62.1	34.3	4.365	-208.117	-266.637	-266.637
8	1428.9	1452.1	75.4	170	40	78.3	36.6	4.858	-158.358	-220.555	-220.555
9	1583.4	1614.5	96.3	619	140	76.6	36.3	20.264	-198.352	-257.594	-257.594
10	1683.7	1713.6	53.9	194	38	103.3	41.7	5.798	-316.143	-366.68	-366.68
11	1737.6	1771.9	79	454	98	103.3	41.7	15.975	-248.513	-304.048	-304.048
12	1817.9	1843	54.5	133	27	108.4	43.3	3.585	-297.508	-349.422	-349.422
13	1912.1	1941.6	91.3	532	120	79.5	37.5	16.858	-200.95	-260	-260
14	2073.5	2108.7	125.2	502	114	64	33.6	19.906	-198.71	-257.925	-257.925
15	2233.2	2285.2	128.4	2032	450	58.2	32.2	73.151	-214.278	-272.343	-272.343
16	2394.1	2437.4	110.4	1307	292	80.7	37.2	44.978	-208.775	-267.247	-267.247
17	2546	2600	149	2090	464	62.2	33.2	78.601	-213.827	-271.925	-271.925
18	2697.6	2737.9	98.8	870	197	77.4	36.5	34.852	-201.811	-260.797	-260.797
19	2840.3	2909.9	146.5	3063	704	89.2	38.8	134.503	-201.053	-260.096	-260.096
20	2987.4	3034.7	130.6	1382	317	121.5	46.9	57.915	-201.079	-260.119	-260.119
21	3119.3	3213.8	132.1	4581	1091	96.7	41	252.351	-204.145	-262.959	-262.959
22	3251.4	3258.5	22.6	719	180	96.7	41	12.623	-219.8	-277.457	-277.457
23	3274	3317.2	112.9	2251	505	96.7	41	83.073	-263.482	-304.482	-304.482
24	3387.5	3460.4	118.1	3170	740	143.8	51.4	148.531	-197.473	-256.779	-256.779
25	3505.6	3527.9	40.3	538	113	143.8	51.4	15.46	-242.061	-298.073	-298.073
26	3545.9	3627.4	97.2	2215	468	143.8	51.4	109.032	-249.235	-304.716	-304.716
27	3643.1	3671.5	94.7	1469	334	143.8	51.4	54.398	-206.255	-264.913	-264.913
28	3749	3789.2	83.4	977	206	163.6	55.2	29.045	-237.582	-293.924	-293.924
29*	3849.2	3873.4	68.6	272	82	113.7	43.8	8.124	-176.2	-237.079	-237.079
30*	3959.5	4026.3	120.6	2998	899	138.7	50.3	125.043	0	-244.1	-244.1
31	4996.4	4997.2	102	1652	286	46.5	30.3	155.564	-299.937	-470.822	-470.822
32	5115.7	5116.7	62.5	1634	267	33.3	26.2	93.887	-295.334	-467.343	-467.343
Duplicate 2											
1	19.4	20.3	22.2	1811	264	33.1	26.4	30.66	-436.775	-478.398	-478.398
2	99.1	99.9	22.2	1617	264	33.2	26.3	30.626	-436.547	-478.186	-478.186
3	198.6	199.6	22.4	1593	263	33.2	26.4	30.771	-437.05	-478.652	-478.652
4	298	299.1	22.2	1598	262	33.2	26.5	30.51	-437.221	-478.811	-478.811
5	509.3	530	100.9	2327	654	38.2	27.5	51.357	-24.402	-96.499	-96.499
6*	1143	1187.5	134	5873	1699	68	35.3	171.862	0	-73.9	-73.9
7	1263.7	1303.7	65	171	39	63.5	34.2	4.541	-193.218	-252.839	-252.839
8	1429.8	1453.4	75.2	175	41	80.5	37.6	5.053	-191.783	-251.51	-251.51
9	1583.8	1616.2	96.6	639	145	78.7	36.6	21.13	-199.179	-258.36	-258.36
10	1685	1714.6	53.7	199	38	107.4	42.8	6.006	-325.873	-375.691	-375.691
11	1738.7	1773.4	79	472	102	107.4	42.8	16.643	-253.206	-308.394	-308.394
12	1818.9	1844.8	54.5	138	29	112.2	43.7	3.723	-278.831	-332.125	-332.125
13	1913.4	1943.7	104.1	555	125	81.9	36	17.486	-203.19	-262.074	-262.074
14	2074.7	2108.8	125.4	521	119	65.6	33.6	20.7	-195.197	-254.672	-254.672
15	2234.4	2287.3	127.3	2092	465	59.5	32.3	75.993	-214.529	-272.575	-272.575
16	2395.6	2439.7	117.5	1360	304	83.1	37.8	46.699	-210.668	-269	-269
17	2547.5	2602.3	149	2159	479	63.9	33.4	79.611	-213.174	-271.32	-271.32
18	2699	2740.4	96.3	905	206	79.8	36.1	36.047	-194.115	-253.67	-253.67
19	2842	2912.4	146.7	3135	722	92.1	39.2	138.818	-201.149	-260.184	-260.184
20	2989.3	3037.8	130.6	1454	334	126.3	47.5	60.036	-198.789	-257.998	-257.998
21	3121.2	3216.9	132.5	4701	1120	100.5	41.2	260.956	-203.293	-262.169	-262.169
22	3253.7	3261.7	23	748	167	100.5	41.2	13.572	-217.206	-275.054	-275.054
23	3276.7	3319.8	112.7	2310	519	100.5	41.2	85.621	-202.234	-261.169	-261.169
24	3390	3462.9	117.5	3247	758	147.3	52.3	152.399	-197.873	-257.15	-257.15
25	3507.4	3529.8	39.9	575	120	147.3	52.3	16.08	-242.69	-298.655	-298.655
26	3547.4	3630.3	98.4	2276	461	147.3	52.3	112.283	-249.463	-304.928	-304.928
27	3645.8	3673.6	92	1499	341	147.3	52.3	55.659	-207.058	-265.656	-265.656
28	3750.3	3791.3	94.9	999	211	164	55.2	29.898	-237.714	-294.047	-294.047
29	3850.4	3879.2	79.2	247	57	113.4	44	8.788	-185.717	-245.893	-245.893
30*	3960.6	4029.9	121.4	2981	895	140.1	50.4	123.609	0	-244.1	-244.1
31	4261.1	4304.6	64.2	51	12	93.2	39.7	1.856	77.351	-185.631	-185.631
32	4996.4	4997.2	101.8	1462	234	48	30.7	137.819	-302.719	-472.926	-472.926
33	5115.7	5116.7	62.3	1437	236	33.2	26.2	83.332	-297.625	-469.075	-469.075

2422

Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (V)	rd T (permil) vs. C18	dT (permil) vs. C18	dD (permil) vs. VSMOW
Duplicate 1											
1	19.4	20.3	21.9	1453	233	34.2	25.9	27.324	-441.801	-482.886	-482.886
2	99.1	99.9	21.9	1449	233	34.2	25.7	27.288	-440.755	-482.083	-482.083
3	198.6	199.4	21.9	1449	233	34.3	25.4	27.413	-440.119	-481.495	-481.495
4	298	298.9	21.9	1431	232	34.9	25.7	27.2	-441.532	-482.803	-482.803
5	508.5	529.6	106	3110	857	45.9	29.3	68.89	-24.865	-96.742	-96.742
6*	1139.6	1169.8	122.7	2188	827	52	30.9	54.488	0	-73.9	-73.9
7	1279.1	1300	66	132	32	59.5	32.7	3.577	-149.993	-212.809	-212.809
8	1427.7	1450.3	71.5	147	36	81.1	37	3.657	-132.928	-197.005	-197.005
9	1580.7	1613.3	89	573	131	73.3	35.4	16.856	-189.481	-249.378	-249.378
10	1674.1	1705.2	60.6	164	31	91.6	40	4.947	-335.127	-384.261	-384.261
11	1735.1	1789.2	76.3	465	102	117.2	44.3	14.447	-235.254	-291.789	-291.789
12	1813.1	1844.2	95.7	193	39	106.7	42.6	4.296	-297.067	-349.014	-349.014
13	1910.1	1945.2	86.5	823	185	70.8	34.7	23.945	-199.892	-259.02	-259.02
14	2074.7	2110.3	119.3	869	153	83.8	38.1	20.969	-215.48	-273.456	-273.456
15	2232.1	2291.9	132.5	2640	596	63	32.9	99.295	-197.558	-260.563	-260.563
16	2395.1	2435.9	107	1182	296	77.5	36	35.901	-207.054	-265.652	-265.652
17	2545.2	2600.8	122.3	2217	499	83.6	32.5	78.919	-194.332	-253.871	-253.871
18	2698.4	2737.1	94.3	883	200	84.5	37.4	27.214	-200.628	-258.701	-258.701
19	2838.8	2900.5	145	2490	571	83.5	37.3	67.791	-195.637	-255.079	-255.079
20	2884.7	3028.4	101.2	1117	254	119.2	45.6	35.884	-202.307	-261.256	-261.256
21	3115.4	3192.1	112	3068	714	92.5	39.5	141.244	-237.711	-294.045	-294.045
22	3227.4	3240.5	35.5	855	142	92.5	39.5	15.868	-206.619	-265.25	-265.25
23	3282.9	3296.6	105.3	1283	286	92.5	39.5	39.244	-196.42	-255.805	-255.805
24	3374.1	3442.6	110.1	2479	577	105.7	41.5	101.995	-322.474	-372.543	-372.543
25	3484.9	3510.4	42	353	89	299.4	87.6	6.162	-234.269	-290.856	-290.856
26	3526.9	3544.8	35.1	304	86	299.4	87.6	4.702	-308.08	-359.213	-359.213
27	3562	3592.7	52	854	130	299.4	87.6	14.327	-204.521	-263.307	-263.307
28	3614	3670.7	118.5	1134	259	299.4	87.6	30.776	-251.174	-308.512	-308.512
29	3733.2	3780	104.1	841	137	126.2	47	83.6	-173.722	-234.784	-234.784
30	3841.8	3879.2	78.8	386	88	83.6	36.6	10.55	0	-244.1	-244.1
31*	3956	4016.1	117.9	1950	448	93.8	38.8	73.584	-312.146	-480.051	-480.051
32	4995.9	4997	101.8	1341	213	44.4	29	126.681	-307.437	-476.492	-476.492
33	5115.5	5116.3	61.9	1322	216	34.1	25.6	76.505			
Duplicate 2											
1	19.4	20.5	21.9	1311	213	34.1	25.2	25.066	-440.907	-482.224	-482.224
2	99.1	100.1	21.9	1307	212	34.1	25.7	25.031	-442.893	-484.064	-484.064
3	198.6	199.6	22.2	1314	212	34.1	25.6	25.149	-442.266	-483.483	-483.483
4	298	299.1	21.9	1319	212	34.1	25.2	24.951	-441.525	-482.796	-482.796
5	508.5	530.4	106.2	3317	945	44.1	28.7	73.537	-28.365	-100.189	-100.189
6*	1139.7	1169.8	121.8	2369	679	51.1	30.4	58.209	0	-73.9	-73.9
7	1279.9	1298.5	64.6	155	37	58.9	31.9	3.861	-131.517	-195.688	-195.688
8	1429.4	1448.8	99.6	178	43	81.4	37.9	3.988	-208.902	-249.903	-249.903
9	1574.6	1612.6	90.5	692	156	73	35	17.559	-190.047	-249.903	-249.903
10	1677.4	1705.2	58.5	192	37	91.9	39.7	5.377	-335.57	-384.671	-384.671
11	1736.6	1772.3	75.9	535	118	110.5	42.3	15.898	-235.086	-291.622	-291.622
12	1813.5	1843.8	68.1	254	51	101.2	41.6	5.729	-310.874	-361.893	-361.893
13	1911.9	1945.6	80.9	973	215	88.3	34.1	25.095	-201.416	-260.431	-260.431
14	2076.6	2110.5	115.4	825	184	80.2	37.4	22.383	-204.854	-263.615	-263.615
15	2234.4	2296.1	132.9	2674	802	82.2	32.3	103.21	-214.025	-272.109	-272.109
16	2397.6	2439.4	108.7	1283	285	77	36	37.245	-203.209	-262.082	-262.082
17	2547.9	2606.2	127.1	2214	496	85.6	33.1	82.045	-194.099	-268.889	-268.889
18	2701.1	2740.8	92	1008	225	84.7	37.4	28.106	-199.895	-253.855	-253.855
19	2841.1	2906.8	129	2455	558	84.5	37.5	98.793	-259.023	-263.655	-263.655
20	2987.7	3035.1	108.1	1189	286	126.1	47	36.086	-194.047	-259.607	-259.607
21	3118.5	3201.5	148.5	3109	715	97.1	40.1	159.87	-203.276	-262.154	-262.154
22	3285	3308.9	107	1183	263	97.1	40.1	39.82	-201.098	-260.137	-260.137
23	3374.9	3457.5	123.7	2346	540	109.9	43.1	105.273	-197.357	-256.672	-256.672
24	3496.3	3522.9	42.2	259	50	356.5	99.9	3.46	-382.672	-428.292	-428.292
25	3541.5	3558.4	37	303	66	356.5	99.9	3.804	-237.508	-293.856	-293.856
26	3578.5	3605.9	49.5	582	113	356.5	99.9	11.005	-322.398	-372.473	-372.473
27	3628	3683	112.4	1162	285	356.5	99.9	25.975	-187.532	-247.573	-247.573
28	3741.1	3794	105.3	648	136	141.2	50.1	19.079	-245.86	-301.405	-301.405
29	3849.6	3887.2	78.8	404	93	89.9	38.3	10.509	-179.354	-240	-240
30*	3958.9	4024.1	126.9	2044	487	101	41	74.921	0	-244.1	-244.1
31	4996.1	4997	101.6	1228	195	44.3	28.5	116.328	-309.85	-478.185	-478.185
32	5115.7	5116.5	61.9	1233	196	33.9	25.6	70.305	-305.957	-475.373	-475.373
Duplicate 3 (C40)											
1	19.4	20.5	21.9	1379	229	27.3	8.8	26.254	-435.931	-494.199	-494.199
2	99.1	100.1	21.9	1375	229	27.3	9	26.22	-436.36	-494.584	-494.584
3	198.6	199.6	22.2	1385	229	27.3	9.1	26.326	-436.407	-494.626	-494.626
4	298	299.1	21.9	1392	229	27.4	8.8	26.131	-435.416	-493.738	-493.738
5	1137.4	1146.8	49.7	1367	38	37.2	11.2	2.421	-39.222	-138.47	-138.47
6	1274.7	1284.9	26.5	53	13	40	11.6	0.828	-152.856	-240.386	-240.386
7	1422.7	1432.3	51	71	17	46.1	12.9	1.363	-132.471	-222.086	-222.086
8	1578.2	1593.4	63.7	313	69	47.7	13.3	5.742	-189.71	-273.413	-273.413
9	1665.9	1696.8	57.7	72	15	51.2	13.9	1.95	-273.328	-348.393	-348.393
10	1724.9	1753.3	68.6	219	49	52.9	14.5	5.832	-239.62	-318.167	-318.167
11	1809.3	1821	39.5	97	20	68.5	17.9	1.316	-296.915	-369.544	-369.544
12	1804.4	1822.8	66.5	459	100	44.3	12.5	6.706	-192.73	-278.121	-278.121
13	2087.6	2085.8	53.9	421	92	44.5	12.6	7.772	-191.595	-275.103	-275.103
14	2227.7	2282.8	104.5	1394	299	42.5	12.2	35.814	-298.095	-374.979	-374.979
15	2385.9	2406.1	72.3	632	138	45.9	12.4	12.923	-191.456	-274.979	-274.979
16	2538.3	2570.5	97.6	1115	240	44.8	12.5	27.245	-212.958	-294.26	-294.26
17	2687.5	2708	71.7	480	101	48.7	13.2	9.045	-190.18	-273.834	-273.834
18	2830.9	2884.1	105.1	1124	245	48.1	13.4	28.743	-203.486	-285.786	-285.786
19	2972.2	2993.1	70.2	484	107	53.5	14.5	9.581	-191.184	-274.735	-274.735
20	3108.2	3141.9	62.7	1158	255	50.4	13.6	27.796	-201.622	-284.094	-284.094
21	3170.9	3188.6	67.9	325	71	50.4	13.8	9.275	-226.833	-308.315	-308.315
22	3236.7	3256.8	50	320	71	62.9	16.5	5.687	-196.100	-279.151	-279.151
23	3350.3	3392.3	89	641	142	59.1	15.7	15.6	-202.854	-285.019	-285.019
24	3440.3	3484.2	54.8	210	43	80.3	20.8	4.49	-272.591	-347.733	-347.733
25	3495.5	3504.9	31.8	62	15	79	19.8	0.746	-113.192	-204.8	-204.8
26	3528.3	3551.7	49.5	393	79	78.1	20.1	7.889	-269.255	-344.741	-344.741
27	3578.3	3588.9	32.2	72	15	127.7	31.2	0.502	-333.448	-402.301	-402.301
28	3610.5	3625.9	61.2	168	40	127.7	31.2	0.674	-109.789	-4.87	-4.87
29	3701.6	3739.2	85.3	314	66	63.8	16.8	6.582	-243.225	-321.4	-321.4
30*	4385.2	4433.3	79.2	800	219	56.1	15.5	23.613	-103.3	-103.3	-103.3
31	4484.4	4478.8	56.6	45	15	56.1	15.5	3.339	-78.372	-78.372	-78.372
32	4995.5	4996.6	101.6	1271	209	38.5	11.9	121.039	-439.259	-497.184	-497.184
33	5115.1	5115.9	61.9	1289	211	27.4	8.5	73.152	-435.601	-493.904	-493.904
Duplicate 4											
1	19.4	20.5	21.9	1619	270	26.8	9	30.84	-436.601	-494.8	-494.8
2	99.1	100.1</									

2422 CONT

8	1574 4	1600 7	86 3	653	149	67 3	18 4	17 59	-188 016	-271 894	-271 894
9	1682 6	1690 2	59 4	180	35	84 5	22 6	5 325	-327 083	-306 596	-306 596
10	1722	1757 5	74 6	512	113	84 5	22 6	17 697	-248 998	-326 577	-326 577
11	1797 8	1826 3	102	218	44	105 8	27 7	4 174	-366 899	-432 298	-432 298
12	1900 6	1931 6	82 6	1001	224	61 9	17 2	26 599	-198 437	-281 238	-281 238
13	2064 7	2095 6	112 9	820	187	73 2	20 4	24 132	-199 98	-281 725	-281 725
14	2223 1	2281 7	127 1	3028	685	56 5	15 9	110 483	-218 731	-299 436	-299 436
15	2385 5	2422 9	101 8	1505	333	68 3	18 7	40 787	-202 481	-284 847	-284 847
16	2536	2589 9	118 5	2585	580	60 4	17	89 214	-216 581	-297 49	-297 49
17	2688 2	2722 9	91 1	1143	257	78 2	20 6	31 383	-193 52	-276 829	-276 829
18	2829 4	2890 1	148 3	2894	696	79 8	21 3	112 318	-206 554	-288 517	-288 517
19	2974 7	3015	95 9	1511	342	79 6	21 3	45 441	-198 563	-281 351	-281 351
20	3108 2	3183 5	110 1	3641	848	89 7	23 3	165 81	-210 346	-291 918	-291 918
21	3218 4	3227 4	33	738	163	89 7	23 3	15 044	-234 412	-313 497	-313 497
22	3251 4	3285 7	103 9	1555	345	89 7	23 3	45 125	-203 006	-285 336	-285 336
23	3361 6	3433 9	111 8	2835	658	111 3	28 3	116 088	-204 515	-286 688	-286 688
24	3474 2	3497 8	41 8	321	62	383 9	91 9	3 943	-380 387	-444 393	-444 393
25	3516	3533 8	33 9	391	83	383 9	91 9	3 509	-190 131	-273 791	-273 791
26	3549 9	3580 2	51	769	151	383 9	91 9	14 073	-310 305	-381 55	-381 55
27	3600 9	3611 5	19 6	172	29	383 9	91 9	1 499	-430 393	-489 233	-489 233
28	3620 5	3657 3	95 9	1447	330	383 9	91 9	27 992	-178 31	-261 397	-261 397
29	3726 5	3764 5	96 6	785	165	143 4	35 8	20 178	-250 682	-328 086	-328 086
30	3825 5	3859 6	70 4	519	119	84 1	21 5	12 048	-174 883	-260 117	-260 117
31	4043 1	4055 5	38 7	58	14	82 1	16 8	0 998	-107 592	-199 778	-199 778
32	4380 2	4433 1	83 6	645	231	68 8	18 8	27 263	0	-103 3	-103 3
33	4483 8	4473 6	52 7	127	37	68 8	18 8	2 358	68 588	-41 797	-41 797
34	4995 9	4996 8	101 6	1497	245	45 5	13 9	141 425	-439 735	-497 81	-497 81
35	5115 5	5116 3	61 9	1512	247	26 8	9	85 748	-436 726	-494 912	-494 912

2522

Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (vs)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs. VSMQW
Duplicate 1											
1	19.4	20.5	21.7	839	134	28.4	22	15.918	-445.797	-486.752	-486.752
2	99.1	99.9	21.7	849	134	28.5	22	15.901	-445.428	-486.411	-486.411
3	198.6	199.6	21.9	837	134	28.4	22.3	15.968	-447.413	-488.25	-488.25
4	298	299.1	21.9	839	134	28.4	21.9	15.96	-445.015	-486.029	-486.029
5	441.2	449.6	47	92	26	29.8	22.1	6.624	8.009	-66.483	-66.483
6*	1078.3	1093.5	80.9	1076	298	31.6	23	19.472	0	-73.9	-73.9
7	1422.9	1430.2	21.1	89	21	37.3	23.9	1.051	-188.489	-229.938	-229.938
8	1524	1533.9	44.1	98	21	52.3	27.6	1.455	-243.261	-299.184	-299.184
9	1579	1585.7	45.8	59	13	44.9	25.9	0.807	-246.734	-302.4	-302.4
10	1628.3	1637.7	59.6	269	60	40.7	24.7	4.22	-184.908	-245.143	-245.143
11	1724.5	1733.2	55.2	190	43	38.2	24.3	3.014	-184.536	-244.798	-244.798
12	1817	1831.7	57.7	787	169	37.7	24.1	13.552	-213.595	-271.71	-271.71
13	1906.5	1915.9	55.2	264	58	44.5	25.8	4.036	-209.887	-268.277	-268.277
14	1991.8	2005.8	62.9	702	152	39.1	24.4	12.095	-212.591	-270.781	-270.781
15	2075	2083.9	42.6	224	50	43.9	25.3	3.309	-193.806	-253.384	-253.384
16	2154.2	2188	58.3	988	146	41.7	24.7	11.902	-202.403	-251.345	-251.345
17	2232.3	2241.7	47.7	277	61	52.6	27.4	4.052	-194.667	-254.181	-254.181
18	2305.9	2326.2	57.1	1505	335	45.7	25.7	29.238	-197.75	-257.037	-257.037
19	2363	2368.2	17.6	150	34	45.7	25.7	1.842	-196.47	-255.851	-255.851
20	2380.5	2386.9	45.1	324	72	45.7	25.7	5.399	-202.492	-261.428	-261.428
21	2449.3	2454.5	64	678	150	52.1	26.6	12.473	-186.19	-246.33	-246.33
22	2518.8	2524.5	40.1	148	32	75.5	32.6	1.984	-251.887	-307.173	-307.173
23	2554.8	2573.8	30.3	526	106	64.5	29.5	6.836	-272.761	-326.504	-326.504
24	2585.1	2591.2	55.6	436	95	64.5	29.5	7.263	-211.719	-269.973	-269.973
25	2644.9	2652	19.6	78	18	85.5	30.1	0.877	-182.436	-242.854	-242.854
26	2664.5	2672.7	40.3	158	33	85.5	30.1	2.351	-242.786	-296.744	-296.744
27*	2771.3	2804.6	100.5	2206	499	80.9	29	54.327	0	-244.1	-244.1
28	3482.8	3483.8	31.8	805	128	28.8	22.2	22.821	-306.171	-475.535	-475.535
29	3582.3	3583.3	32	809	127	28.4	22.2	22.689	-307.025	-476.16	-476.16
Duplicate 2											
1	19.4	20.3	21.7	804	127	28.5	22.2	15.08	-446.305	-487.223	-487.223
2	99.1	99.9	21.7	811	127	28.5	22	15.064	-445.675	-486.64	-486.64
3	198.6	199.4	21.9	802	127	28.5	22	15.14	-445.082	-486.09	-486.09
4	298	299.1	21.7	792	126	28.5	22	15.023	-445.428	-486.411	-486.411
5	440.8	449.6	58.3	234	64	29.8	22.4	4.051	-33.832	-105.046	-105.046
6*	1075.3	1096.6	92.6	1786	498	32.3	23.2	35.014	0	-73.9	-73.9
7	1422.5	1426.6	20.9	88	21	37.3	24	1.047	-171.805	-233.009	-233.009
8	1523.4	1533.2	44.1	98	21	52.4	27.5	1.448	-231.968	-288.448	-288.448
9	1578.4	1585.1	43.9	59	13	45	25.6	0.812	-199.613	-258.782	-258.782
10	1627.7	1637.1	59.4	266	59	40.8	24.7	4.199	-183.991	-244.294	-244.294
11	1723.8	1732.6	54.5	187	42	38.3	24.2	2.961	-175.151	-236.107	-236.107
12	1816.4	1831	57.7	777	168	37.7	23.9	13.365	-208.658	-267.138	-267.138
13	1905.9	1915.3	55.2	263	58	44.5	25.4	4.004	-187.697	-247.726	-247.726
14	1990.9	2005.1	63.1	699	150	39.2	24.3	12.048	-209.225	-267.664	-267.664
15	2074.1	2083.1	42.8	223	49	43.9	25.6	3.311	-203.428	-262.295	-262.295
16	2153.3	2167.3	58.3	664	146	41.7	24.5	11.808	-196.802	-256.158	-256.158
17	2231.5	2240.9	47.9	275	60	52.5	27.7	4.036	-212.988	-271.149	-271.149
18	2305.3	2325.5	57.1	1492	332	45.5	25.7	28.96	-195.732	-255.167	-255.167
19	2362.3	2368.4	17.3	149	34	45.5	25.7	1.859	-195.708	-255.145	-255.145
20	2379.7	2388	45.1	323	71	45.5	25.7	5.315	-200.25	-259.351	-259.351
21	2448.6	2462.9	64	674	149	51.9	27	12.441	-194.965	-254.457	-254.457
22	2512.6	2523.9	40.3	170	37	51.9	27	2.923	-222.474	-279.933	-279.933
23	2554	2573.2	30.3	522	105	64.4	29.8	6.767	-261.384	-334.49	-334.49
24	2584.3	2590.6	58.9	433	94	64.4	29.8	7.241	-217.821	-275.624	-275.624
25	2644.3	2652	21.2	121	27	85	30.1	1.349	-200.859	-259.916	-259.916
26	2664.3	2672.1	40.3	164	35	85	30.1	2.471	-249.248	-304.729	-304.729
27*	2770.5	2812.9	118.3	3218	741	59.2	28.4	93.86	0	-244.1	-244.1
28	3482.8	3483.8	31.8	758	121	28.8	22.2	21.628	-306.047	-475.441	-475.441
29	3582.3	3583.3	32	761	121	28.4	22	21.691	-305.092	-474.719	-474.719
Duplicate 3											
1	19.4	20.5	21.9	1310	215	32.8	26.1	25.1	-442.737	-483.919	-483.919
2	99.1	100.1	22.2	1313	214	32.9	26	25.031	-442.647	-483.835	-483.835
3	198.6	199.6	22.4	1314	213	32.9	26.1	25.167	-442.901	-484.071	-484.071
4	298	299.1	22.2	1321	213	33	25.9	24.954	-441.943	-483.183	-483.183
5	506.4	524.4	109.9	808	224	41.7	28.8	29.895	-28.176	-99.994	-99.994
6*	1142	1170.2	107.8	2484	705	41.3	28.3	59.185	0	-73.9	-73.9
7	1429.1	1441.3	48.7	85	17	52.7	31.1	1.377	-108.652	-174.523	-174.523
8	1585.1	1602.6	61.7	295	65	56.6	31.9	6.387	-185	-245.228	-245.228
9	1675.3	1702.5	60.8	254	48	66	34.2	6.51	-324.889	-374.78	-374.78
10	1738.8	1754.8	69.6	278	61	78.5	36.8	6.749	-248.228	-303.784	-303.784
11	1808.3	1835.6	63.7	208	42	64.7	33.9	3.891	-285.456	-338.26	-338.26
12	1913	1938.7	96.8	785	171	52.2	31.1	18.104	-208.877	-267.341	-267.341
13	2076.8	2099.8	96.1	571	126	51.4	30.6	12.866	-195.323	-254.788	-254.788
14	2237.6	2282.1	146.7	1809	393	41.2	29.8	56.985	-219.347	-277.038	-277.038
15	2396.5	2424.8	74.6	724	158	72.1	35.2	15.997	-206.385	-265.033	-265.033
16	2549.4	2592.4	103.7	1628	354	50.4	30.4	48.769	-220.662	-278.255	-278.255
17	2701.1	2726.2	74.4	636	139	57.1	31.5	14.098	-198.51	-257.74	-257.74
18	2843.2	2865.7	109.7	1541	340	55	31.2	48.506	-212.49	-270.687	-270.687
19	2987.4	3014.4	86.3	753	164	67.5	34.3	17.295	-207.914	-266.45	-266.45
20	3121.8	3168.8	141.3	2934	670	59.5	32.2	124.593	-208.319	-266.824	-266.824
21	3263.5	3290.3	84.6	748	163	65.3	38.4	17.288	-218.634	-276.377	-276.377
22	3377.4	3433.7	97.8	1472	331	74.2	35.3	47.724	-205.003	-263.753	-263.753
23	3475.7	3496.5	55.4	157	30	158.3	56	2.599	-430.239	-472.344	-472.344
24	3531.7	3547.8	28.8	237	52	93.2	39.7	3.49	-208.453	-285.096	-285.096
25	3560.5	3599.8	60.4	1181	237	93.2	39.7	34.296	-285.432	-338.238	-338.238
26	3620.9	3623.9	16.1	306	65	93.2	39.7	3.774	-273.918	-327.576	-327.576
27	3637	3659	65	675	150	93.2	39.7	16.505	-202.924	-261.828	-261.828
28	3740.1	3773.5	79.8	421	88	93.4	39.4	9.734	-248.694	-304.216	-304.216
29	3841.4	3870.9	49.3	126	30	71.6	34.7	2.853	-192.707	-252.366	-252.366
30*	3962.2	3968	98.3	1000	225	84.6	36.8	26.069	0	-244.1	-244.1
31	4985.9	4986.8	101.8	1202	190	43.3	29.2	113.141	-320.589	-486.433	-486.433
32	5115.3	5116.3	62.3	1189	191	33	26.3	68.309	-317.112	-483.805	-483.805
Duplicate 4											
1	19.4	20.5	22.2	1169	190	33	25.9	22.363	-440.789	-482.115	-482.115
2	99.1	100.1	21.9	1184	190	33	25.9	22.312	-440.71	-482.041	-482.041
3	198.6	199.6	22.2	1172	189	32.9	26.1	22.408	-441.718	-482.975	-482.975
4	298	299.1	22.2	1177	188	32.9	26.1	22.216	-442.014	-483.249	-483.249
5	508.9	530.7	102.4	2743	776	38.4	28.1	61.236	-27.141	-99.035	-99.035
6*	1141.6	1189.8	129.8	6457	1961	58	32.9	209.956	0	-73.9	-73.9
7	1283.9	1300	61.7	61	15	57.4	33	1.674	-157.573	-219.828	-219.828
8	1421.8	1449.8	65.4	112	28	64.7	34.6	2.945	-149.258	-212.128	-212.128
9	1574.5	1611.2	85.9	394	88	69.7	35.7	12.949	-199.358	-258.525	-258.525
10	1671.2	1708.4	86.5	367	70	100.7	42.1	11.911	-325.653	-375.487	-375.487
11											

2522 CONT

16	2392 2	2433 8	106	1186	263	87 3	39 1	33 672	-202 926	-261 829	-261 829
17	2546 5	2605 6	121 8	2646	596	66 7	34 2	99 791	-213 337	-271 471	-271 471
18	2700 3	2735 4	81 9	964	220	85 6	38 7	28 132	-200 64	-259 713	-259 713
19	2840 7	2892 2	118 9	2463	560	83 2	37 8	97 562	-205 177	-263 914	-263 914
20	2986 4	3023	95 9	941	216	130 1	48 7	32 422	-196 855	-256 208	-256 208
21	3116	3209 2	153 6	4418	1057	94	40	250 678	-197 993	-256 984	-256 984
22	3269 6	3300 3	103	1312	292	94	40	40 334	-201 905	-260 964	-260 964
23	3379 1	3448 5	108 9	1961	455	108 6	43 6	98 318	-196 901	-255 672	-255 672
24	3488 4	3506 6	43 1	170	32	338	98 5	3 358	-395 186	-439 685	-439 685
25	3548 8	3613 2	93	1754	361	258 6	78 1	71 132	-277 908	-331 271	-331 271
26	3641 8	3670 5	75 2	696	196	258 6	78 1	26 168	-197 021	-256 361	-256 361
27	3736 3	3785 2	104 5	614	129	144 2	51 5	21 086	-249 524	-304 984	-304 984
28	3843 5	3890 5	62 1	190	44	101 7	41 8	5 632	-195 233	-254 706	-254 706
29	3956 8	4033 5	134 6	3254	771	125 1	46 7	148 636	0	-244 1	-244 1
30	4996 1	4997 2	101 8	1066	168	46 1	30 1	100 537	-311 377	-479 47	-479 47
31	5115 7	5116 7	62 1	1047	170	33	26 1	60 932	-304 522	-474 288	-474 288

2600

Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs. VSMOW
Duplicate 1											
1	19.4	20.3	21.9	977	154	32.6	26	18.385	-444.27	-485.339	-485.339
2	99.1	99.9	21.9	974	154	32.6	25.7	18.35	-442.83	-484.005	-484.005
3	198.6	199.4	21.9	970	154	32.6	26.2	18.422	-445.269	-486.263	-486.263
4	298	298.9	21.9	952	153	32.7	25.9	18.265	-443.727	-484.835	-484.835
5	509.1	531.7	104.1	3056	868	36.2	27.7	99.009	-27.363	-99.241	-99.241
6*	1141.8	1193.4	139.6	6924	2107	53.9	32.1	235.443	0	-73.9	-73.9
7	1818.4	1831.5	49.5	70	15	43.8	28.8	1.338	-250.2	-305.611	-305.611
8	1913	1927.2	56.4	150	35	42.8	28	2.784	-126.279	-190.847	-190.847
9	2078.2	2090.6	52.5	133	32	42.2	27.7	2.494	-85.571	-153.147	-153.147
10	2236.7	2280.8	69.4	544	119	41.5	28.4	11.689	-192.73	-252.387	-252.387
11	2395.6	2411.9	65.6	228	52	52.4	30.8	4.328	-176.51	-237.366	-237.366
12	2547.1	2572.4	93.2	569	127	41.7	27.7	12.838	-173.624	-234.693	-234.693
13	2696.7	2713.4	58.9	195	45	44.4	28.5	3.707	-134.583	-198.538	-198.538
14	2840.1	2865.6	53.7	552	123	43.9	28.4	11.588	-176.406	-237.27	-237.27
15	2893.8	2899	38.7	70	17	43.9	28.4	1.588	-157.255	-219.534	-219.534
16	2981.8	2998.3	65.2	196	45	49.4	29.9	3.894	-158.04	-220.261	-220.261
17	3115.8	3144.8	67.5	693	155	45	28.4	16.646	-174.795	-235.777	-235.777
18	3249.3	3265.6	46	182	42	51.4	30.1	3.307	-164.842	-217.299	-217.299
19	3353.2	3401.9	99.5	563	125	51.1	29.5	13.859	-170.986	-232.231	-232.231
20	3455	3475.3	47.7	65	14	71.9	34.5	1.109	-201.413	-260.429	-260.429
21	3503.5	3514.8	34.9	51	13	58.9	31.7	0.747	-110.97	-176.669	-176.669
22	3539.8	3558.2	47.9	148	31	58.3	31.9	2.859	-256.882	-311.78	-311.78
23	3619	3633.5	36.8	89	21	57.5	31.3	1.498	-141.553	-204.992	-204.992
24	3729.8	3750.9	64.8	229	51	62.9	32.7	4.44	-190.8	-250.6	-250.6
25*	3956.4	4039.6	162.4	3530	823	64.2	32.9	168.963	0	-244.1	-244.1
26	4995.5	4996.6	101.6	880	138	40.5	28	83.09	-309.674	-478.183	-478.183
27	5115.1	5116.1	61.9	863	139	32.6	25.7	50.174	-305.627	-475.123	-475.123
Duplicate 2											
1	19.4	20.3	21.9	862	137	32.6	26	16.411	-445.625	-486.593	-486.593
2	99.1	99.9	21.9	864	136	32.6	26	16.38	-445.695	-486.658	-486.658
3	198.6	199.6	21.9	855	137	32.6	25.6	16.446	-443.914	-485.009	-485.009
4	298	299.1	21.9	859	136	32.7	26.1	16.308	-446.449	-487.356	-487.356
5	508.7	531.9	106.4	3378	965	38.7	27.7	76.858	-26.924	-98.835	-98.835
6*	1141.8	1195.3	142.3	7432	2275	56.1	32.8	259.198	0	-73.9	-73.9
7	1818	1830.6	49.7	87	15	43.7	28.5	1.285	-228.83	-285.82	-285.82
8	1912.1	1926.4	57.5	144	33	42.8	28.4	2.674	-180.41	-222.456	-222.456
9	2075.4	2089.8	52.5	127	31	42.1	28	2.38	-114.981	-180.384	-180.384
10	2236.1	2259.7	69.2	524	116	41.5	28.1	11.195	-187.995	-248.003	-248.003
11	2384.9	2411	66	220	52	51.9	30.1	4.149	-139.718	-203.293	-203.293
12	2546.5	2571.3	93.4	549	121	41.5	28	12.285	-163.865	-244.177	-244.177
13	2695.9	2712.6	57.5	198	44	44.1	28.4	3.552	-140.85	-204.341	-204.341
14	2839.7	2864.6	53.3	533	120	43.7	28.1	11.127	-171.525	-232.75	-232.75
15	2893	2898.4	38.9	67	16	43.7	28.1	1.527	-151.918	-214.591	-214.591
16	2981	2997.3	64.8	188	44	49	29.5	3.537	-142.831	-206.176	-206.176
17	3114.9	3143.6	66.9	668	149	44.8	28.5	15.883	-178.636	-236.335	-236.335
18	3248.7	3264.8	45.6	175	41	50.7	29.9	3.172	-162.602	-224.485	-224.485
19	3351.9	3400.8	99.9	544	121	50.5	29.6	13.309	-180.618	-241.17	-241.17
20	3454.1	3474.4	47.7	63	14	70.4	34.2	1.075	-220.754	-278.341	-278.341
21	3539.2	3557.4	47.7	142	30	57.4	31.6	2.75	-262.906	-317.378	-317.378
22	3618.6	3632.8	37	85	22	56.1	29.3	1.447	2.692	-71.407	-71.407
23	3729	3750.9	65.6	239	53	62.1	32.7	4.712	-201.508	-260.517	-260.517
24*	3956	4042.7	162.8	3713	870	63	32.5	182.879	0	-244.1	-244.1
25	4995.7	4996.6	101.6	784	123	40	28	74.23	-313.73	-481.249	-481.249
26	5115.1	5116.1	61.9	783	123	32.5	25.7	44.85	-308.434	-477.245	-477.245
Duplicate 3 (C40)											
1	19.4	20.5	21.9	1180	195	27.3	8.2	22.485	-435.37	-493.696	0.0000789 -493.696
2	99.1	100.1	21.9	1177	194	27.4	9	22.455	-438.395	-496.408	0.0000784 -496.408
3	198.6	199.6	21.9	1187	194	27.4	8.7	22.54	-437.449	-495.561	0.0000786 -495.561
4	298	299.1	21.9	1191	194	27.4	8.8	22.379	-437.416	-495.531	0.0000786 -495.531
5	1138	1148.2	53.3	102	29	35.3	10.3	2.067	9.702	-94.6	0.000141 -94.6
6	1579	1590.5	59.6	134	31	47	13.4	2.523	-191.913	-275.388	0.0001129 -275.388
7	1864.5	1878.1	59.1	104	21	52.7	14.6	2.569	-295.986	-368.711	0.0000983 -368.711
8	1724.9	1752.5	69.2	121	27	56	15.3	2.976	-213.737	-294.958	0.0001098 -294.958
9	1806.8	1822.3	52.7	214	43	57.4	15.8	3.789	-292.504	-365.588	0.0000988 -365.588
10	1904.6	1923	65.6	474	106	54.6	14.3	8.922	-164.6	-250.897	0.0001167 -250.897
11	2067.8	2086.2	55.2	426	97	54.4	15	8.029	-166.683	-252.747	0.0001164 -252.747
12	2228.4	2285.1	74.4	1478	322	51.8	14.4	37.68	-203.84	-285.904	0.0001112 -285.904
13	2388.7	2410.8	90.1	685	153	86.3	22.1	13.541	-169.952	-255.696	0.0001159 -255.696
14	2538.5	2577	99.5	1520	334	51.7	14.4	41.517	-202.793	-285.144	0.0001113 -285.144
15	2688.6	2711.4	74	597	135	59.2	15.9	12.143	-165.541	-251.741	0.0001165 -251.741
16	2831.7	2870	80.4	1469	328	56.5	15.1	36.836	-193.73	-277.018	0.0001126 -277.018
17	2892.1	2894.4	36.2	310	73	56.5	15.1	5.785	-199.418	-282.118	0.0001118 -282.118
18	2974.7	2996.6	80	610	137	72.6	18.9	12.238	-169.452	-255.248	0.0001116 -255.248
19	3109.3	3152.6	74.8	1813	407	59.8	15.7	54.515	-196.623	-278.612	0.0001122 -278.612
20	3184.1	3187	30.5	414	96	56.8	16.7	8.094	-222.21	-302.555	0.0001086 -302.555
21	3214.6	3218	28.6	115	27	59.8	15.7	2.001	-196.725	-282.394	0.0001118 -282.394
22	3243.3	3264.6	61.7	587	132	59.8	15.7	13.654	-182.191	-266.67	0.0001142 -266.67
23	3345.7	3409.2	103.5	1499	334	82.2	20.2	44.691	-196.436	-279.444	0.0001122 -279.444
24	3449.5	3473.8	50.8	152	30	179.4	45	2.333	-396.496	-458.838	0.0000843 -458.838
25	3500.3	3512.5	34.3	109	24	179.4	45	-0.181	76.844	-34.394	0.0001504 -34.394
26	3535.2	3559.7	50.2	468	94	110.2	27.7	9.1	-269.5	-344.961	0.000102 -344.961
27	3585.4	3593.1	26.1	93	20	110.2	27.7	1.191	-278.886	-353.377	0.0001007 -353.377
28	3611.5	3628.7	39.1	282	64	110.2	27.7	4.309	-269.225	-329.225	0.0001138 -329.225
29	3674.2	3687.6	28.2	56	12	98.1	25.1	0.997	-252.767	-329.957	0.0001044 -329.957
30	3721.9	3741.1	61.7	279	60	110.5	27.2	4.351	-219.144	-299.806	0.0001091 -299.806
31	3838.9	3849.8	30.1	53	14	102.3	24.8	0.505	-221.189	-301.822	0.0001088 -301.822
32	3892.6	3908.7	29.7	67	15	91.5	23.2	1.219	-157.646	-244.661	0.0001176 -244.661
33	3948.6	3960.3	51.2	77	18	86.6	22.3	1.035	0	-103.3	0.0001397 -103.3
34*	4386.3	4435.4	79.4	843	230	63.7	17	25.89	52.656	-56.084	0.0000777 -56.084
35	4465.7	4477.8	56.6	162	46	63.7	17	3.181	-443.377	-500.876	0.0000776 -500.876
36	4995.5	4996.6	101.6	1105	177	43.1	13.3	103.295	-443.377	-500.876	0.0000776 -500.876
37	5115.1	5116.1	61.9	1084	179	27.4	8.5	62.704	-437.401	-495.518	0.0000786 -495.518
Duplicate 4 not enough											

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Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (permil) vs. C18	dT (permil) vs. C18	dD (permil) vs. V8MOW
Duplicate 1											
1	19.4	20.3	21.7	836	130	28.5	22.3	15 538	-465 655	-505 143	-505 143
2	99.1	99.9	21.7	834	130	28.5	22.2	15 505	-465 303	-504 817	-504 817
3	198.6	199.4	21.9	827	130	28.5	22.1	15 576	-464 783	-504 317	-504 317
4	298	299.1	21.7	816	130	28.5	21.9	15 484	-463 496	-503 144	-503 144
5	538.4	553.6	70.2	262	74	32.1	23.2	5 735	-21 878	-94 161	-94 161
6*	1163.1	1181.5	83.2	911	262	33.6	23.4	18 415	0	-73.9	-73.9
7	1361.5	1408.2	46.6	75	19	45	26.1	1 445	-122.89	-187 708	-187 708
8	1504.6	1517.5	81.7	306	72	55	28.3	5 734	-172 551	-233.7	-233.7
9	1567.1	1578.4	37.8	74	18	65.1	30.6	1 332	-270 823	-324 801	-324 801
10	1605.3	1621.4	55	383	87	72.5	32.4	6 783	-211 983	-270 217	-270 217
11	1680.7	1669.9	39.3	118	25	80	34.3	1 693	-302 339	-353 896	-353 896
12	1709.2	1729.1	87.4	1442	323	67.9	31.4	29 236	-234 027	-290 833	-290 833
13	1804.1	1823.1	87.4	1173	266	67	31	23 373	-217 412	-275 245	-275 245
14	1882.9	1931.8	95.7	4171	968	66.5	30.3	111 249	-273 347	-327 046	-327 046
15	1988.6	2008.7	81.9	1647	372	66.5	30.3	34 891	-228 188	-285 224	-285 224
16	2071	2104.4	86.1	3691	851	78	33.5	94 407	-268 724	-322 786	-322 786
17	2157.1	2176.3	76.7	1582	356	78	33.5	33 29	-232 199	-288 94	-288 94
18	2233.8	2270.6	82.3	4353	1027	78	33.5	121 108	-271 382	-325 227	-325 227
19	2318.1	2335.8	74	1904	435	78	33.5	42 846	-230 237	-287 122	-287 122
20	2390.1	2431.1	69	5716	1596	78	33.5	163 919	-283 898	-336 633	-336 633
21	2459.1	2485.4	53.7	2004	460	78	33.5	54 89	-237 548	-293 893	-293 893
22	2512.8	2581.5	89.5	3237	761	78	33.5	88 34	-244 272	-300 12	-300 12
23	2602.3	2614.6	43.7	1113	247	78	33.5	21 173	-242 036	-298 05	-298 05
24	2646.4	2679.8	79	1255	285	229.8	68.5	28 792	-248 213	-303 77	-303 77
25	2725.4	2733.7	19.4	67	15	229.8	68.5	0 197	-213 122	-271 273	-271 273
26	2744.8	2781.1	40.1	510	107	229.8	68.5	7 298	-288 416	-341 002	-341 002
27	2784.9	2792.9	18	149	34	229.8	68.5	1 315	-234 951	-291 488	-291 488
28	2802.9	2807.3	44.7	62	13	229.8	68.5	-2.01	-188 636	-248 596	-248 596
29*	2847.6	2867.1	69.6	738	170	229.8	68.5	7 932	0	-244.1	-244.1
30	3483	3484	31.8	784	122	29.7	22.4	22 033	-347 168	-506 524	-506 524
31	3582.7	3583.5	31.8	787	122	28.5	22.1	22 111	-348 707	-506 178	-506 178
Duplicate 2											
1	19.4	20.5	21.7	879	139	28.3	22.3	16 625	-442 101	-483 33	-483 33
2	99.1	100.1	21.7	876	139	28.4	22.1	16 603	-440 958	-482 271	-482 271
3	198.6	199.6	21.9	882	138	28.4	22.4	16 671	-442 265	-483 482	-483 482
4	298	299.1	21.9	888	138	28.4	22.5	16 547	-442 325	-483 538	-483 538
5	540.7	559.9	91.1	1241	352	31.2	23	27 361	6 281	-68 102	-68 102
6*	1165.2	1187.4	113.3	3653	1079	39.5	25.6	92 403	0	-73.9	-73.9
7	1367.6	1413.7	49.1	100	25	53.5	28.3	2 241	-87 625	-155 05	-155 05
8	1505.2	1523.2	63.7	374	87	67	31.7	8 505	-150 339	-213 129	-213 129
9	1569.8	1586.5	37.2	86	18	66.6	36.4	1 896	-269 634	-323 808	-323 808
10	1607.4	1627.3	53.7	458	103	102.6	36.5	9 456	-182 089	-242 533	-242 533
11	1661.6	1678.8	47.2	129	26	109.6	41.7	2 076	-307 402	-358 585	-358 585
12	1709.2	1733.4	93.8	1895	427	89.8	38.6	42 526	-200 881	-259 751	-259 751
13	1804.5	1829	91.3	1445	331	79.6	34.4	34 492	-182 11	-242 553	-242 553
14	1898.5	1938.3	94.1	5474	1312	80.9	33.9	181 57	-250 646	-306 023	-306 023
15	1990.5	2013.7	81.7	2186	501	80.9	33.9	50 133	-190 838	-250 835	-250 835
16	2072.2	2110.9	86.9	4674	1114	80.9	33.9	133 055	-232 486	-289 205	-289 205
17	2159.2	2181.8	75.7	2034	469	80.9	33.9	47 903	-183 371	-243 72	-243 72
18	2234.8	2277.7	83.8	5461	1330	80.9	33.9	168 335	-236 298	-292 736	-292 736
19	2318.6	2342.1	70	2499	564	80.9	33.9	82 521	-184 041	-244 341	-244 341
20	2388.7	2440.9	81.9	6637	1657	80.9	33.9	240 288	-247 329	-302 951	-302 951
21	2470.6	2492.1	50.4	2684	630	80.9	33.9	73 87	-196 308	-255.7	-255.7
22	2521	2567.8	84.6	4097	988	80.9	33.9	123 875	-202 799	-261 712	-261 712
23	2605.6	2621.5	41.8	1403	315	80.9	33.9	29 844	-186 589	-248 552	-248 552
24	2647.4	2683.8	81.5	1844	426	80.9	33.9	58 171	-185 854	-255.28	-255.28
25	2728.9	2785.7	58.3	906	196	80.9	33.9	25 144	-194 659	-254 174	-254 174
26	2787.2	2795.6	80.4	447	103	80.9	33.9	13 552	-163 232	-225 069	-225 069
27*	2847.6	2864.6	87.8	3675	881	80.9	33.9	122 629	0	-244.1	-244.1
28	2935.8	2937.5	18.6	178	45	80.9	33.9	2 256	144 361	-134 977	-134 977
29	3325.8	3372.8	73.2	66	16	66.9	30.6	1 855	103 694	-165 717	-165 717
30	3483.4	3484.2	31.8	842	131	30	22.8	23 555	-264 389	-466 629	-466 629
31	3582.9	3583.9	32	825	130	28.6	22.5	23 642	-264 376	-466 619	-466 619
Duplicate 3											
1	19.4	20.5	21.9	858	104	32.4	25.7	12 571	-447 51	-488 339	-488 339
2	99.1	100.1	21.9	857	104	32.4	25.8	12 542	-447 764	-488 574	-488 574
3	198.6	199.6	21.9	859	103	32.4	26	12 594	-449 863	-490 518	-490 518
4	298	299.1	21.9	862	103	32.4	25.9	12 499	-447 945	-488 742	-488 742
5	510.4	535.5	111.2	4096	1176	39.5	28.2	95 987	-27 425	-99 298	-99 298
6*	1142.6	1202.9	145.5	8770	2746	68.6	36	332 863	0	-73.9	-73.9
7	1431.4	1447.1	48.3	51	14	43.6	28.1	1 135	-5 097	-78 621	-78 621
8	1585.9	1605.5	65.2	144	33	45.6	29.2	3 469	-186 291	-246 424	-246 424
9	1734.1	1788.8	70	161	37	49.4	29.7	4 36	-195 147	-254 626	-254 626
10	1817.3	1837.7	51	51	11	49.4	29.7	1 198	-244 477	-300 31	-300 31
11	1909.2	1940.1	92.2	717	157	46.4	29	18 682	-207 385	-265 959	-265 959
12	2072.9	2104	95.1	529	118	46.8	29.3	14 85	-196 691	-256 056	-256 056
13	2233.4	2284	118.7	2145	475	45.4	28.7	70 754	-213 802	-271 995	-271 995
14	2394.5	2426.9	92.4	798	175	51.2	30.1	21 207	-204 917	-262.84	-262.84
15	2545.6	2593.9	116.2	1898	418	47.6	29	60 523	-210 974	-269 283	-269 283
16	2696.9	2729.5	89.5	753	160	52.8	30.1	20 403	-195 67	-255.11	-255.11
17	2838.6	2863.6	120.4	2200	494	63.9	30.1	77 515	-203 122	-262 012	-262 012
18	2983.5	3018	93.6	918	203	66.1	33.1	25 228	-195 506	-254 958	-254 958
19	3116	3181.8	104.9	2737	628	59.3	31.6	112 175	-199 133	-258 317	-258 317
20	3257.5	3286.7	112	911	198	103	41.9	22 318	-212 709	-270 89	-270 89
21	3371.8	3422.2	95.3	1565	354	70.3	33.7	49 653	-189 179	-249 099	-249 099
22	3466.1	3491.1	41.2	194	38	129.5	48.9	3 125	-336 956	-385 955	-385 955
23	3509.3	3526.2	39.3	214	46	129.5	48.9	3 373	-247 478	-303 09	-303 09
24	3548.6	3570.3	45.6	224	43	129.5	48.9	3 957	-349 472	-397 268	-397 268
25	3594.6	3609.4	27.6	68	14	122.5	45.5	9 965	-288 691	-341 256	-341 256
26	3622.2	3647.1	71.5	452	102	122.5	45.5	8 946	-185 326	-227 009	-227 009
27	3718.1	3758.7	95.7	502	109	70.2	33.7	11 836	-211 154	-269.45	-269.45
28	3836.2	3870.7	89.5	103	24	56.1	30.9	3 259	-187 479	-247 524	-247 524
29*	3852.6	4045.8	169.1	4159	987	59	31.5	217 739	0	-244.1	-244.1
30	4895.9	4997	101.6	598	93	40.3	27.7	56 883	-316 357	-483 234	-483 234
31	5115.5	5116.3	61.7	605	94	32.5	25.6	34 49	-312 694	-480 465	-480 465
Duplicate 4											
1	19.4	20.5	21.7	592	93	32.5	25.3	11 305	-449 285	-489 883	-489 883
2	99.1	100.1	21.7	594	93	32.6	25.1	11 271	-448 263	-489 037	-489 037
3	198.6	199.6	21.9	594	93	32.6	25.3	11 325	-449 985	-490 631	-490 631
4	298	299.1	21.9	596	93	32.6	25.3	11 239	-449 812	-490 471	-490 471
5	507.9	528.8	40.5	2072	579	38.4	26.9	43 996	-39 257	-110 256	-110 256
6	548.4	556.1	83.2	1063	304	38.4	26.9	31 086	-5 343	-78 848	-78 848
7*	1142.6	1184	12								

13	2395.6	2420	76.3	564	123	44.8	27.5	12.054	-194.794	-254.299	-254.299
14	2547.3	2585.5	101.4	1271	275	42.5	27.1	34.526	-211.799	-270.047	-270.047
15	2698.6	2722.6	75.2	540	117	45.7	27.9	11.663	-201.912	-260.891	-260.891
16	2841.1	2883.8	109.7	1509	331	46.2	27.6	44.593	-204.622	-263.401	-263.401
17	2984.5	3010.9	87.8	652	143	52.2	29.1	14.735	-197.655	-256.948	-256.948
18	3119.3	3169.9	136.7	1955	436	48.1	28.1	68.808	-202.083	-261.05	-261.05
19	3256.8	3281.1	86.5	602	131	60.7	31.1	14.399	-212.534	-270.728	-270.728
20	3370.5	3416.7	93.8	1046	233	55.3	29.3	28.841	-190.127	-249.676	-249.676
21	3485.4	3487.2	44.3	126	25	81.6	36.7	2.218	-337.003	-385.998	-385.998
22	3509.7	3523.5	39.5	153	33	81.6	36.7	2.3	-258.05	-312.88	-312.88
23	3549.9	3567	44.5	175	36	84.2	36	0.921	-272.722	-326.468	-326.468
24	3595.2	3608	28.8	52	11	83.6	35.7	2.922	-270.373	-324.293	-324.293
25	3624.5	3643.7	64.8	325	73	81.7	35.2	0.892	-169.992	-231.329	-231.329
26	3729.2	3755.3	76.7	282	61	58.6	29.7	5.811	-200.944	-259.994	-259.994
27	3838.7	3863.4	47.2	76	19	49.7	27.7	1.596	-139.811	-203.379	-203.379
28*	3956.4	4011.5	119.5	1950	442	51.8	28.3	67.363	0	-244.1	-244.1
29	4996.7	4996.8	101.6	544	84	40.4	26.4	51.279	-324.15	-489.125	-489.125
30	5115.3	5116.1	61.7	546	85	32.7	24	31.123	-316.71	-483.501	-483.501

Triplicate 1

1	19.2	38.7	23.2	797	133	257.7	92.5	15.64	-415.332	-458.539	-458.539
2	99.1	100.3	23.2	794	132	259.6	93.3	15.548	-416.255	-459.393	-459.393
3	198.6	213	21.9	794	132	257.7	93.2	15.659	-418.58	-461.547	-461.547
4	298.2	302.6	21.7	793	131	258.9	93.5	15.529	-419.294	-462.208	-462.208
5	368.3	371.2	16.7	1434	102	258	93.4	3.216	-696.087	-718.546	-718.546
6	911.7	916.9	13.4	55	16	205.6	94.8	0.292	82.359	2.373	2.373
7*	948	971.6	44.5	8312	2287	266.4	95	96.486	0	-73.9	-73.9
8	1193.4	1199.9	13.2	132	33	267	95.7	0.582	-80.026	-148.012	-148.012
9	1333.6	1341.2	19.6	499	114	268.2	95.8	2.492	-127.504	-191.981	-191.981
10	1385.7	1391.1	13.8	99	23	270.3	95.6	0.504	-165.539	-227.206	-227.206
11	1440.2	1446.5	15	116	26	270.8	96.2	0.585	-181.146	-241.66	-241.66
12	1480.6	1490.4	23.6	528	118	268.7	95.3	2.969	-129.447	-193.781	-193.781
13	1514.2	1520.9	18.2	172	37	275.2	96.6	0.848	-199.81	-258.944	-258.944
14	1635.4	1653.2	43.5	1633	311	267.4	94.9	15.168	-167.75	-229.253	-229.253
15	1792.4	1807.8	43.9	1165	245	270	95.6	12.009	-153.711	-216.252	-216.252
16	1949.3	1983.6	51	3478	706	271.7	96.1	57.395	-195.518	-254.969	-254.969
17	2104.2	2124.7	45.1	1401	300	273.7	95.8	17.486	-162.267	-224.176	-224.176
18	2253.9	2289.8	55	3029	623	272.5	95.6	49.419	-190.422	-250.25	-250.25
19	2403.9	2424.8	44.7	1274	277	275.8	97	16.491	-157.704	-219.95	-219.95
20	2545.6	2586.4	54.1	3450	708	278.8	98.9	62.856	-182.931	-243.311	-243.311
21	2687.3	2713	42.4	1608	338	287.6	98.9	20.704	-163.751	-225.55	-225.55
22	2822.3	2870.2	56.4	3649	783	279.3	96.6	90.433	-179.627	-240.253	-240.253
23	2878.8	2883.4	19.4	113	24	279.3	96.6	1.24	-215.247	-273.24	-273.24
24	2947.7	2982.8	47	1595	330	289.5	99.1	21.556	-168.914	-230.332	-230.332
25	3024	3038.9	25.3	160	36	288.3	98.2	1.658	-192.739	-252.396	-252.396
26	3086.1	3120.8	40.1	2463	514	291.8	99.1	40.294	-154.867	-217.323	-217.323
27	3126.2	3131.7	28.8	487	99	291.8	99.1	4.303	-265.163	-319.468	-319.468
28	3206.7	3227	36.8	1027	225	295.2	99	10.763	-177.285	-238.066	-238.066
29	3246.8	3261.4	29.3	216	48	284.4	96.3	2.466	-180.465	-241.029	-241.029
30	3335.8	3358.1	32.4	1128	236	275.5	94.9	11.065	-335.451	-399.341	-399.341
31	3396.3	3416.1	31.4	654	126	295.2	99.4	6.384	-201.461	-260.473	-260.473
32	3455.2	3465.6	23.8	153	37	275.1	94.5	1.147	-108.189	-174.094	-174.094
33	3508.9	3517.1	19.9	70	16	277.8	95.5	0.506	-182.572	-242.98	-242.98
34	3573.7	3583.9	23	267	64	275	94.7	1.955	-108.774	-174.636	-174.636
35	3687.8	3696.2	19.9	72	18	273.8	94.3	0.573	-91.406	-158.551	-158.551
36	3799.4	3807.6	17.6	56	14	273.1	94.2	0.429	-112.896	-178.453	-178.453
37	4996.6	5003.5	101.6	742	123	259	93.5	73.239	-419.405	-462.311	-462.311
38	5116.1	5134.9	62.3	738	122	258.1	93.2	43.892	-418.982	-461.919	-461.919

Triplicate 2

1	17.8	32.2	23.4	732	121	258.2	93.3	14.367	-417.08	-460.157	-460.157
2	99.1	110.8	23	732	122	257.6	92.9	14.357	-415.04	-458.269	-458.269
3	198.6	205.7	21.9	731	121	257.8	93.3	14.364	-418.279	-461.288	-461.288
4	298.2	306	22.2	729	121	257.8	93.2	14.291	-417.115	-460.19	-460.19
5	910.4	915.4	14	59	17	264.4	95.2	0.341	-19.482	-91.942	-91.942
6*	946.1	970.8	51.8	8598	2397	264.8	94.8	103.13	0	-73.9	-73.9
7	1192.3	1198.2	12.3	131	33	266.8	95.2	0.581	-51.218	-121.333	-121.333
8	1331.1	1339.3	20.5	479	110	268.9	95.8	2.466	-122.184	-187.054	-187.054
9	1384	1389.4	13.2	96	21	270.5	95.9	0.477	-175.99	-236.885	-236.885
10	1438.1	1444.6	15	105	25	271.1	94.4	0.552	-64.725	-84.725	-84.725
11	1479.1	1488.1	33.2	401	95	268.6	94.3	3.004	-85.851	-153.407	-153.407
12	1512.3	1518.8	18.2	168	39	266.6	94.3	0.973	-119.206	-184.297	-184.297
13	1632.1	1650.3	44.7	1449	295	269.2	95	15.072	-160.384	-222.432	-222.432
14	1789.5	1805.3	48.3	931	212	270.7	95.9	12.076	-152.434	-215.089	-215.089
15	1946	1982.4	53.7	3511	700	271	95.5	57.933	-152.67	-252.331	-252.331
16	2102.3	2123.4	42.6	1504	312	275.5	96.7	17.478	-164.389	-226.14	-226.14
17	2253.2	2288.1	55	3008	619	273.2	96.2	49.758	-189.335	-249.243	-249.243
18	2400.6	2423.6	41	1390	295	279.2	96.8	16.643	-159.156	-221.295	-221.295
19	2543.7	2582.6	55	3167	702	272.1	94.9	62.743	-180.038	-240.633	-240.633
20	2598.7	2605.4	19	64	14	272.1	94.9	0.796	-199.034	-258.226	-258.226
21	2686.5	2712	49	1648	343	287	98.6	20.703	-159.189	-221.325	-221.325
22	2819	2867.3	58.5	3607	807	277.7	96.1	90.734	-176.666	-237.511	-237.511
23	2877.5	2882.3	19.4	116	25	277.7	96.1	1.255	-195.084	-254.587	-254.587
24	2946.5	2981.6	47.4	1608	329	287.3	99.1	21.792	-188.527	-229.973	-229.973
25	3020.7	3037.4	24.9	182	40	287.2	97.9	1.659	-168.377	-229.834	-229.834
26	3064.6	3076.1	20.3	53	15	286.1	98.2	0.483	-167.187	-228.732	-228.732
27	3084.8	3120.2	41	2516	515	285.1	98.2	41.01	-152.392	-215.031	-215.031
28	3125.8	3130.6	29.5	506	100	286.1	98.2	4.269	-270.379	-324.298	-324.298
29	3205.6	3225.5	37.4	1039	228	297.5	99.7	10.819	-175.384	-236.323	-236.323
30	3244.9	3260.8	31.1	225	49	283.6	96.5	2.539	-188.312	-248.295	-248.295
31	3335.4	3395.1	32.6	1157	240	275.1	95.3	11.312	-138.505	-202.17	-202.17
32	3395.4	3416.1	32	653	128	294.7	99.6	6.548	-200.394	-258.485	-258.485
33	3455.2	3465.8	21.1	159	38	275.3	94.6	1.172	-103.455	-169.71	-169.71
34	3508.9	3517.3	18.4	71	16	277.3	95.3	0.498	-124.31	-189.023	-189.023
35	3571	3584.1	25.5	277	67	274.4	93.6	2.017	-55.966	-125.73	-125.73
36	3688.6	3697.2	23.8	76	19	274.7	94.8	0.602	-104.845	-170.997	-170.997
37	3799.4	3808.8	21.7	56	15	274.3	93.7	0.425	-102.356	-20.892	-20.892
38	4996.6	5001.6	101.4	683	113	256.6	93.3	67.499	-418.068	-461.073	-461.073
39	5116.1	5124.5	61.7	677	112	259	93.9	40.237	-419.411	-462.316	-462.316

Triplicate 3

1	19.4	23.6	23	673	112	257	93.4	13.198	-416.523	-459.642	-459.642
2	99.1	115.2	22.8	673	111	256.8	93.4	13.206	-416.798	-459.896	-459.896
3	198.6	216.5	23.8	670	111	258.8	93.4	13.212	-414.044	-457.347	-457.347
4	298.2	306.7	21.5	670	110	257.7	93.9	13.116	-420.161	-463	

2722 CONT

16	2100.2	2120.9	44.7	1562	335	276.4	97.6	19.806	-165.408	-227.084	-227.084
17	2250.3	2287.1	57.7	3001	653	273.1	95.5	55.945	-184.381	-244.655	-244.655
18	2399.1	2421.5	45.4	1433	309	280.6	98.4	18.656	-161.557	-223.518	-223.518
19	2541.6	2583.9	55.6	3275	692	273.7	96.7	67.955	-177.603	-238.378	-238.378
20	2597.2	2602.7	20.3	68	15	273.7	96.7	0.884	-217.771	-275.578	-275.578
21	2684	2710.1	41.2	1754	360	291.7	100.5	23.203	-156.193	-218.551	-218.551
22	2818.4	2868.7	59.5	3867	841	280.4	97.5	102.025	-176.447	-237.308	-237.308
23	2876.9	2880.6	18.8	136	30	280.4	97.5	1.345	-173.209	-234.309	-234.309
24	2945.4	2980.8	48.3	1697	358	289.3	99.9	24.601	-163.871	-225.661	-225.661
25	3018	3035.7	27.4	192	42	286.9	99.4	1.95	-201.916	-260.894	-260.894
26	3062.7	3073.8	20.1	53	12	288.3	99.9	0.499	-180.852	-241.387	-241.387
27	3082.8	3120	42.8	2726	560	288.3	99.9	46.714	-153.231	-215.897	-215.897
28	3125.6	3129.8	28	569	110	288.3	99.9	4.373	-271.551	-325.383	-325.383
29	3204.4	3224.7	35.1	1156	251	299.7	102	12.414	-185.069	-245.292	-245.292
30	3243.7	3260	31.6	251	56	286	97.8	2.872	-181.335	-241.834	-241.834
31	3335	3355.5	31.8	1254	259	276.2	98.4	12.993	-137.693	-201.39	-201.39
32	3394.2	3415.5	32	724	140	302.1	101.8	7.479	-195.863	-255.289	-255.289
33	3455	3464.4	18.9	180	44	279.4	96.5	1.321	-118.047	-183.223	-183.223
34	3506.8	3515.6	18.8	85	20	279.7	97	0.627	-183.234	-243.593	-243.593
35	3567.4	3583.1	28	308	72	274.5	95.7	2.325	-107.355	-173.322	-173.322
36	3685.3	3694.3	20.9	85	21	273.1	95.4	0.669	-82.725	-150.512	-150.512
37	3792.5	3806.1	27	67	17	271.8	94.9	0.55	-66.93	-135.884	-135.884
38	4696.6	5004.7	101.6	631	105	256	94.1	62.39	-417.895	-460.913	-460.913
39	5115.7	5120.3	62.3	628	103	257.7	94.4	37.311	-418.196	-461.191	-461.191

	T1	T2	T3	average	stdev
C23	-254.969	-252.331	-253.984	-253.7613333	1.333021505
C25	-250.25	-249.243	-244.855	-248.0493333	2.98238769
C27	-243.311	-240.633	-238.378	-240.774	2.469520804
C29	-240.253	-237.511	-237.308	-238.3573333	1.644830184

	T1	T2	T3
C16	948	946.1	945.1
C23	1983.6	1982.4	1981.5
C25	2289.8	2288.1	2287.1
C27	2586.4	2582.6	2583.9
C29	2870.2	2867.3	2868.7
C36	4033	4033	4033

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Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (permil) vs. C16	dT (permil) vs. C16	dD (permil) vs. VSMCW
Duplicate 1											
1	19.4	20.3	21.7	499	78	32.8	22.7	9.483	-448.088	-488.875	-488.875
2	99.1	99.9	21.7	500	79	32.7	22.3	9.447	-444.973	-485.989	-485.989
3	198.6	199.6	21.9	493	78	32.7	22.6	9.481	-447.896	-488.697	-488.697
4	298	299.1	21.7	495	78	32.7	22.7	9.408	-448.418	-489.18	-489.18
5	510.4	538.2	118.1	5286	1537	41.6	25.2	129.822	-27.392	-99.287	-99.287
6*	1143.4	1210.3	150.7	10298	3287	71.7	33.6	425.021	0	-73.9	-73.9
7	3732.7	3751.1	60	153	36	38.2	22.6	3.081	-115.564	-180.924	-180.924
8*	3955.7	4030.6	156.1	3096	698	43.7	24.5	129.983	0	-244.1	-244.1
9	4995.5	4996.6	101.4	458	71	37.6	23.4	42.965	-318.717	-485.018	-485.018
10	5114.9	5115.9	61.9	460	72	32.8	21.4	26.004	-307.823	-476.783	-476.783
Duplicate 2											
1	19.2	20.3	21.7	448	71	32.8	22.2	8.504	-447.746	-488.558	-488.558
2	98.9	99.9	21.7	445	71	32.8	21.3	8.489	-439.338	-480.771	-480.771
3	198.3	199.4	21.9	447	70	32.8	22.2	8.518	-447.339	-488.181	-488.181
4	297.8	298.9	21.7	448	70	32.9	21.9	8.453	-445.469	-488.449	-488.449
5	510.8	541.5	120.4	7189	2154	44.8	25.5	184.488	-28.815	-100.401	-100.401
6*	1141.3	1222.7	180.2	12879	4285	86	37.1	623.482	0	-73.9	-73.9
7	3732.7	3751.8	63.3	186	44	37.5	22.7	3.774	-141.185	-204.633	-204.633
8*	3938.6	4028.5	170.3	2898	673	40.4	23.6	122.435	0	-244.1	-244.1
9	4995.3	4996.1	101.4	412	64	37.1	23.3	38.724	-320.602	-486.443	-486.443
10	5114.6	5115.7	61.9	408	64	32.8	22.1	23.423	-316.924	-483.663	-483.663

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Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (permil) vs. C18	dT (permil) vs. C18	dD (permil) vs. VSMOW
Duplicate 1											
1	19.4	20.3	21.7	378	59	32.9	22	7.133	-851.441	-877.199	-877.199
2	99.1	99.9	21.7	378	59	32.9	21.7	7.121	-849.431	-875.338	-875.338
3	198.6	199.4	21.9	371	59	33	22.1	7.152	-851.942	-877.963	-877.963
4	298	299.1	21.7	372	58	33	22.3	7.092	-853.834	-878.231	-879.231
5	510	554.1	128.3	14364	4683	63.3	30.7	451.973	-384.737	-439.486	-439.486
6*	1262.4	1264.9	101.4	1148	396	19824.3	7384.6	-1648.838	0	-73.9	-73.9
7	1441.3	1453.8	54.5	159	44	58.8	28.6	3.075	-381.418	-408.607	-408.607
8	1592.2	1607.4	58.1	287	89	74.7	31.9	5.288	-380.927	-426.677	-426.677
9	1751.4	1770	57.5	405	103	92.6	36.9	7.954	-381.258	-426.983	-426.983
10	1914.9	1936.4	63.5	530	132	96.3	39	11.553	-392.147	-437.067	-437.067
11	2018.7	2057.4	65.6	749	181	114.1	43.1	16.793	-395.825	-440.288	-440.288
12	2084.4	2102.5	59.8	555	139	114.1	43.1	12.691	-371.893	-418.31	-418.31
13	2238.6	2267.2	68.1	825	193	107.6	41.8	20.191	-402.81	-446.942	-446.942
14	2396.4	2421.3	75	520	127	133.7	48	11.527	-365.735	-412.807	-412.807
15	2540.8	2578.2	86.5	706	186	115.5	43.3	16.961	-372.877	-419.037	-419.037
16	2695.3	2723.5	60.8	454	110	111.6	42.6	9.882	-346.705	-394.984	-394.984
17	2842.8	2872.7	83.2	891	180	111.6	42.1	16.927	-350.44	-398.442	-398.442
18	2986.2	3009	74.4	446	107	115.4	42.8	10.468	-321.484	-371.627	-371.627
19	3122.5	3154.9	65.4	923	210	117.6	43.6	22.945	-347.431	-395.656	-395.656
20	3188.3	3204	87.5	68	13	220	68.7	-0.651	64.976	-13.726	-13.726
21	3259.8	3276.5	47.9	322	76	137.3	47.8	6.157	-306.406	-359.515	-359.515
22	3374.7	3409.4	88.2	550	125	139.9	48.3	13.865	-325.11	-374.984	-374.984
23	3464	3483.8	46.4	121	26	154.1	52.1	1.977	-414.747	-457.997	-457.997
24	3511	3525	28.6	132	33	130.3	45.8	1.983	-289.811	-323.772	-323.772
25	3540.3	3566.8	53.1	142	29	178.3	57.8	2.105	-406.53	-452.24	-452.24
26	3594.8	3610.1	33.2	72	17	149.2	50	1.013	-316.554	-367.06	-367.06
27	3628.4	3646.4	63.3	295	88	140	48.3	5.418	-287.848	-340.478	-340.478
28	3740.3	3762.8	67.9	434	97	133.1	46.2	8.515	-297.469	-349.386	-349.386
29	3845.4	3873.2	71.1	231	55	109.8	40.2	4.587	-219.222	-278.921	-278.921
30*	3962.8	4033.9	128.5	2963	694	97.1	37.6	126.385	0	-244.1	-244.1
31	4996.1	4997	101.4	348	53	43	24.8	31.985	-330.607	-494.006	-494.006
32	5115.5	5116.5	61.7	343	55	33.4	21.6	19.678	-310.877	-479.092	-479.092
Duplicate 2											
1	19.4	20.3	21.7	342	53	33.3	22.3	6.441	-447.716	-488.53	-488.53
2	99.1	99.9	21.5	341	53	33.4	22.1	6.429	-444.918	-485.939	-485.939
3	198.6	199.4	21.7	341	53	33.4	21.7	6.456	-441.522	-482.794	-482.794
4	298	298.9	21.7	337	53	33.4	22.4	6.404	-448.357	-489.123	-489.123
5	510.4	536.5	112.4	4197	1210	39.9	23.7	98.72	-27.044	-98.946	-98.946
6*	1144.3	1202.2	145.7	8564	2682	61	29.7	318.641	0	-73.9	-73.9
7*	3956.2	3976.2	56.6	225	53	45.7	24.6	4.486	0	-244.1	-244.1
8	4995.3	4996.1	101.4	311	48	38.8	23.5	29.183	-356.973	-513.936	-513.936
9	5114.6	5115.7	61.7	306	49	33.2	22.1	17.78	-351.238	-509.601	-509.601

3822

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Peak number	Start (s)	RT (s)	Width (s)	Ampl. 2 (mV)	Ampl. 3 (mV)	BGD 2 (mV)	BGD 3 (mV)	Area all (Vs)	rd T (permil) vs. C18	dT (permil) vs. C18	dD (permil) vs. VSMCW
Duplicate 1											
1	19 4	20 3	23	4552	814	33 4	24 9	87 033	-431 967	-473 944	-473 944
2	99 1	100 1	22 8	4509	807	33 5	24 9	86 304	-432 251	-474 208	-474 208
3	198 6	199 6	23 2	4504	797	33 5	25 1	85 875	-432 204	-474 164	-474 164
4	298	299 1	23	4495	788	33 6	25 1	84 491	-432 51	-474 447	-474 447
5	506	525 4	96 3	2131	603	37 8	26 2	44 454	-28 409	-100 21	-100 21
6	782 3	793 8	53 1	117	29	36 1	26	2 263	-133 548	-197 577	-197 577
7*	1144 3	1168 9	94 7	1620	462	36 3	25 9	35 045	0	-73 9	-73 9
8	1620 2	1633 5	41 8	89	15	75	33 6	1 612	-248 637	-304 163	-304 163
9	1683 5	1706 3	48 9	167	33	86 2	36 4	4 336	-319 335	-369 636	-369 636
10	1732 4	1772 5	62 9	519	101	88 2	36 4	14 104	-309 829	-360 833	-360 833
11	1795 3	1840 2	108 8	849	164	88 2	36 4	21 653	-312 524	-363 328	-363 328
12	2037 8	2052 2	52	85	22	43 7	27 3	1 626	-79 435	-147 465	-147 465
13	3743 8	3782	47	51	13	56 9	32 1	1 117	-58 77	-128 327	-128 327
14*	3966 4	4020 7	120 4	1844	423	73 3	37 8	81 862	0	-244 1	-244 1
15	4995 5	4996 6	102 2	2714	460	48 4	30 8	257 738	-299 628	-470 588	-470 588
16	5115 1	5115 9	62 5	2697	457	33 5	25 6	153 963	-296 37	-468 126	-468 126
Duplicate 2											
1	19 4	20 3	22 2	2617	439	33 4	25 4	48 983	-434 152	-475 968	-475 968
2	99 1	99 9	22 4	2596	435	33 5	25 5	48 592	-434 248	-476 057	-476 057
3	198 6	199 4	22 4	2540	430	33 5	25 6	48 394	-434 581	-476 366	-476 366
4	298	299 1	22 4	2502	425	33 5	25 6	47 599	-434 829	-476 595	-476 595
5	506 4	526 1	96 6	2185	619	37 9	26 5	45 749	-29 521	-101 239	-101 239
6	782 7	794 2	53 5	121	31	36 1	26	2 348	-120 63	-185 615	-185 615
7*	1144 7	1169 6	94 5	1658	473	36 4	26 2	35 961	0	-73 9	-73 9
8	1620 4	1633 6	42 2	76	16	79	35 1	1 783	-292 344	-344 64	-344 64
9	1683 7	1706 7	49 1	184	35	93 1	37 9	4 777	-335 246	-384 371	-384 371
10	1732 6	1773 6	63 1	566	110	93 1	37 9	15 478	-315 797	-366 36	-366 36
11	1795 9	1841 7	107 4	921	177	93 1	37 9	23 845	-317 174	-367 634	-367 634
12	2037 5	2052 6	52 9	94	24	44 5	27 9	1 776	-96 681	-183 436	-183 436
13	3744 2	3782 2	48 5	51	13	50 8	30 2	1 112	-111 909	-177 539	-177 539
14*	3966 8	4021 6	121 6	1858	426	80 3	33 3	62 731	0	-244 1	-244 1
15	4995 5	4996 4	101 6	1579	255	48 6	30 9	147 328	-306 222	-475 573	-475 573
16	5114 9	5115 9	62 1	1554	264	33 5	25 5	88 376	-299 761	-470 69	-470 69

1626

Peak number	Start time	Retention	Width	Amp2	Amp3	Backgrou	Backgrou	Area all	rD	3H2/2H	d 3H2/2H	d 2H/1H
16ab #1 coinj G												
1	18.8	24.2	22.4	1503	246	863.7	82	29.436	-441.845	-483.093	-483.093	
2	98	106.4	23.4	1487	243	864.9	82.4	29.089	-442.344	-483.554	-483.554	
3	198.1	215.1	22.8	1465	239	863.5	82.3	28.897	-442.422	-483.627	-483.627	
4	298.2	312.9	23.4	1449	235	862.4	82.4	28.379	-443.546	-484.668	-484.668	
5*	842.3	851.3	19.6	1534	365	877.8	63.7	6.948	0	-73.9	-73.9	
6	1207.2	1211.4	7.1	55	12	686.8	66.1	0.197	-179.811	-240.423	-240.423	
7	1214.3	1217.2	10.2	70	15	686.8	66.1	0.304	-214.76	-272.789	-272.789	
8	1338	1343.2	13.6	284	60	685.5	66.1	1.194	-247.984	-303.558	-303.558	
9	1567.1	1573.8	11.9	105	22	698	67.4	0.497	-192.427	-252.107	-252.107	
10	1579	1582.8	11.3	62	14	698	67.4	0.354	-168.921	-230.337	-230.337	
11	1650.7	1659.3	15	562	120	707.5	69.4	3.024	-199.744	-258.863	-258.863	
12	1665.7	1677.4	25.5	95	21	707.5	69.4	1.108	-225.529	-282.763	-282.763	
13	1693.5	1704.8	15	77	17	705.7	69.4	0.43	-221.752	-279.265	-279.265	
14	1713.8	1719.2	13	136	28	723.9	73.2	0.755	-245.02	-300.813	-300.813	
15	1734.9	1740.1	10.4	71	14	725.8	74.4	0.302	-392.423	-437.323	-437.323	
16	1745.4	1750	9.2	84	17	725.8	74.4	0.384	-310.738	-361.675	-361.675	
17	1754.6	1758.1	7.3	81	17	725.8	74.4	0.312	-279.652	-332.886	-332.886	
18	1847.6	1850.9	10.4	80	16	757.2	81.7	0.325	-358.321	-405.741	-405.741	
19	1901.9	1906.7	16.7	61	13	737.4	76	0.539	-264.897	-319.221	-319.221	
20	1918.6	1922.2	18.8	101	21	737.4	76	0.766	-217.952	-275.745	-275.745	
21	1940.1	1946.6	17.6	378	84	726.5	73.7	2.219	-213.534	-271.654	-271.654	
22	2057	2065.5	15.3	101	22	732.3	74.7	0.797	-217.535	-275.359	-275.359	
23	2148.1	2153.7	9.2	142	31	757.5	79.5	0.876	-193.575	-253.169	-253.169	
24	2157.3	2162.9	10.9	305	66	757.5	79.5	1.603	-209.573	-267.886	-267.886	
25	2188.6	2203.7	18.4	785	155	739.4	75	5.357	-204.219	-263.028	-263.028	
26	2207	2208.9	13	194	40	739.4	75	1.13	-241.749	-297.784	-297.784	
27	2245.9	2252.8	12.5	61	13	764.6	80.8	0.245	-179.734	-240.351	-240.351	
28	2301.9	2311.7	14.2	356	77	762.9	80.3	1.892	-183.115	-243.482	-243.482	
29	2316.1	2318.2	6.5	81	18	762.9	80.3	0.403	-210.77	-269.094	-269.094	
30	2322.6	2326.6	10.9	105	23	762.9	80.3	0.559	-178.076	-238.816	-238.816	
31	2342.7	2352.7	23.4	117	24	762	80.9	1.049	-299.788	-351.534	-351.534	
32	2410	2419	15.9	111	24	758.3	80	0.685	-212.795	-270.969	-270.969	
33	3483.2	3486.1	32	962	153	663.7	61.9	28.341	-448.083	-488.87	-488.87	
34	3582.7	3593.5	32.4	949	151	665.5	61.7	28.064	-446.475	-487.381	-487.381	

Ret C16	Ret C36	Ret C36 - F	Ret unknow	Ret unk - Ret C16	Norm ret
842.3	4033	3190.7	1343.2	500.9	0.156987
842.3	4033	3190.7	1659.3	817.9	0.256057
842.3	4033	3190.7	1946.6	1104.3	0.3461
842.3	4033	3190.7	2203.7	1361.4	0.426878
842.3	4033	3190.7	2311.7	1469.4	0.460526

Peak number	Start time	Retention	Width	Amp2	Amp3	Backgrou	Backgrou	Area all	rD	3H2/2H	d 3H2/2H	d 2H/1H
16ab #2 coinj G												
1	18.4	35.3	22.8	917	146	664.7	62	17.916	-445.397	-486.383	-486.383	
2	99.1	109.9	24.7	907	144	664.6	61.7	17.758	-443.377	-484.511	-484.511	
3	198.6	208.6	21.7	893	141	665.5	62.5	17.545	-447.679	-488.495	-488.495	
4	298.2	306	21.7	890	140	663.9	62.2	17.334	-448.009	-488.801	-488.801	
5*	841.4	851	20.7	1499	349	690.1	64.1	6.771	0	-73.9	-73.9	
6	1207.2	1216.8	15	89	17	683.8	65.7	0.859	-285.809	-338.403	-338.403	
7	1338	1343	15.3	332	69	687	66.1	1.373	-247.409	-303.025	-303.025	
8	1372.7	1378.8	11.1	50	9	687.5	66	0.267	-418.319	-461.306	-461.306	
9	1407.8	1413	10.9	54	11	691.4	66.5	0.258	-236.954	-293.343	-293.343	
10	1483.1	1488.1	7.9	63	14	695.3	67.1	0.248	-211.689	-269.927	-269.927	
11	1491	1494.3	13.6	71	14	695.3	67.1	0.459	-260.15	-314.825	-314.825	
12	1569	1573.8	10	128	27	699.3	67.2	0.591	-179.945	-240.547	-240.547	
13	1608	1612	7.5	65	12	716.8	72.2	0.253	-292.704	-344.973	-344.973	
14	1650.7	1659.3	15.5	624	130	713.9	70.4	3.403	-193.01	-252.646	-252.646	
15	1666.1	1677.2	20.9	110	23	713.9	70.4	1.158	-220.717	-278.306	-278.306	
16	1692.7	1704.6	15.9	90	19	710	70	0.512	-244.679	-300.775	-300.775	
17	1713.2	1718.2	8.8	165	35	732	74.8	0.71	-227.508	-284.595	-284.595	
18	1735.5	1739.9	9.6	86	15	736.6	74.7	0.264	-190.051	-174.892	-174.892	
19	1745.2	1749.3	9	82	19	736.6	74.7	0.371	-152.601	-215.224	-215.224	
20	1754.1	1757.9	7.7	85	19	736.6	74.7	0.316	-161.459	-223.427	-223.427	
21	1847.1	1850.5	11.3	83	19	769.6	82.6	0.274	-120.586	-185.575	-185.575	
22	1901.3	1906.7	16.7	70	15	740.2	76.8	0.64	-244.336	-300.18	-300.18	
23	1918	1922.2	20.7	113	24	740.2	76.8	1.022	-295.199	-347.284	-347.284	
24	1940.1	1946.8	18.4	415	93	739.1	74.8	2.439	-199.991	-259.112	-259.112	
25	2042.1	2047.2	10.5	55	11	733.6	74.8	0.258	-280.092	-333.294	-333.294	
26	2056.4	2065.1	14.6	108	24	739.9	76.1	0.879	-216.968	-274.834	-274.834	
27	2110.7	2115.3	10.7	59	12	729.6	73.8	0.325	-263.065	-317.524	-317.524	
28	2140	2145	8.6	52	11	742	75.7	0.283	-225.228	-282.484	-282.484	
29	2148.5	2163.1	19.9	369	79	742	75.7	3.065	-203.373	-262.244	-262.244	
30	2168.4	2170.7	9.6	79	17	742	75.7	0.4	-247.912	-303.491	-303.491	
31	2188.6	2204.1	18.6	855	168	748.1	76.5	5.96	-203.631	-262.483	-262.483	
32	2207.2	2208.9	7.5	220	45	748.1	76.5	1.028	-244.096	-299.958	-299.958	
33	2214.8	2215.6	5.6	53	11	748.1	76.5	0.218	-202.113	-261.077	-261.077	
34	2248.8	2253.2	9	70	14	769.7	82.6	0.3	-276.191	-329.68	-329.68	
35	2299.4	2312	16.9	386	82	771.7	82.2	2.198	-197.943	-257.215	-257.215	
36	2322.6	2326.6	11.7	77	16	813.4	91.3	0.173	-297.315	-349.244	-349.244	
37	2343.9	2352.9	18.4	117	25	773.4	82.8	0.956	-191.959	-251.673	-251.673	
38	2408.7	2419.2	18.8	129	27	765.5	81.6	0.774	-189.503	-249.399	-249.399	
39	2455.1	2459.7	8.6	54	13	759.8	79.7	0.255	-102.881	-169.178	-169.178	
40	3481.5	3490.7	33.4	606	94	662.4	61.5	17.831	-452.594	-493.047	-493.047	
41	3580.2	3589.9	34.7	596	93	665.7	61.6	17.587	-449.697	-490.364	-490.364	

Ret C16	Ret C36	Ret C36 - F	Ret unknow	Ret unk - Ret C16	Norm ret
841.4	4033	3191.6	1343	501.6	0.157163
841.4	4033	3191.6	1659.3	817.9	0.256266
841.4	4033	3191.6	1946.8	1105.4	0.346347
841.4	4033	3191.6	2204.1	1362.7	0.426965
841.4	4033	3191.6	2312	1470.6	0.460772

Peak number	Start time	Retention	Width	Amp2	Amp3	Backgrou	Backgrou	Area all	rD	3H2/2H	d 3H2/2H	d 2H/1H
16ab coinj G 0000												
1	19.4	20.5	22.2	1691	294	329.7	89.3	33.109	-433.314	-475.192	-475.192	
2	99.1	100.1	23.2	1688	293	326.6	89.6	33.05	-434.94	-476.698	-476.698	
3	195.4	198.8	25.3	1681	291	325.4	89.3	33.143	-435.433	-477.154	-477.154	
4	298.2	299.3	21.9	1675	290	324.9	89.1	32.764	-434.602	-476.385	-476.385	
5*	807.7	818.6	27.2	2396	575	331.2	89.9	12.43	0	-73.9	-73.9	
6	1527.2	1533.9	19.9	545	131	335.1	90.8	2.212	-119.901	-184.94	-184.94	
7	1717.1	1722.4	15	97	23	335.6	90.8	0.526	-169.378	-230.761	-230.761	
8	2004.1	2010.2	14.2	60	16	346.7	91.2	0.388	-4.127	-77.722	-77.722	
9	2256.6	2263.7	13.6	201	46	346.1	92.4	0.974	-196.752	-256.112	-256.112	
10	2367.1	2374.9	13.4	53	13	350.6	93.6	0.305	-246.809	-302.285	-302.285	
11	3483.4	3484.7	31.8	1497	258	327.9	89.4	44.158	-435.197	-476.938	-476.938	
12	3582.1	3584.1	33.6	1486	257	325	88.5	44				

16ab CONT

Peak	Trial 1	Trial 2
1	284	332
2	562	624
3	378	415
4	785	855
5	356	386

Peak	Trial 1	Trial 2	Average	St Dev
1	-338.156	-335.049	-336.603	2.196668
2	-283.733	-275.773	-279.753	5.628722
3	-304.422	-290.343	-297.382	9.955228
4	-284.97	-283.02	-283.995	1.378704
5	-278.986	-291.388	-285.187	8.76955

16ac

Peak number	Start time	Retention	Width	Amp2	Amp3	Backrou	Backrou	Area all	rD	3H2/2H	d	3H2/2H	d	2H/1H
230940 16ac #1														
1	19.4	25.5	22.8	577	89	664.4	62.3	11.221	-448.541	-489.294	-489.294			
2	99.1	104.5	21.7	572	89	664.9	61.9	11.099	-445.859	-486.81	-486.81			
3	198.3	218	24.7	564	87	666.5	62.1	11.013	-445.054	-486.074	-486.074			
4	298	306.2	23	557	87	663.6	61.8	10.871	-445.439	-486.421	-486.421			
5*	841.9	851	24	1615	371	676.5	63.7	7.601	0	-73.9	-73.9			
6	1607.8	1613.3	12.1	60	13	677.4	64.9	0.31	-347	-395.257	-395.257			
7	1649.8	1655.3	13.8	121	27	684.5	65.2	0.481	-134.613	-198.565	-198.565			
8	1854.2	1858.2	7.7	78	17	679.9	64.5	0.287	-167.518	-229.039	-229.039	Ret C16	Ret C36	Ret C36 - F
9	2040.5	2054.3	22.4	218	46	682.5	65.4	1.662	-183.31	-243.663	-243.663	Ret C16	Ret C36	Ret C36 - F
10	2138.5	2143.5	9.2	68	15	695.7	67.3	0.304	-137.819	-201.534	-201.534	Ret C16	Ret C36	Ret C36 - F
11	2149.8	2158.6	14.6	122	26	715.7	72.4	0.738	-224.261	-281.588	-281.588	Ret C16	Ret C36	Ret C36 - F
12	2164.4	2167.7	8.4	112	24	715.7	72.4	0.435	-194.637	-254.154	-254.154	Ret C16	Ret C36	Ret C36 - F
13	2178	2182.8	13.2	59	13	714.9	71.6	0.251	-188.241	-248.23	-248.23	Ret C16	Ret C36	Ret C36 - F
14	2262.8	2269.5	13.2	198	43	707.3	69.6	1.041	-203.844	-262.68	-262.68	Ret C16	Ret C36	Ret C36 - F
15	2276	2293.1	21.9	702	136	707.3	69.6	5.427	-223.663	-281.034	-281.034	Ret C16	Ret C36	Ret C36 - F
16	2298	2300	5.2	94	16	707.3	69.6	0.347	-338.317	-387.215	-387.215	Ret C16	Ret C36	Ret C36 - F
17	2303.2	2306.5	6.1	63	12	707.3	69.6	0.298	-356.379	-403.942	-403.942	Ret C16	Ret C36	Ret C36 - F
18	2309.2	2314.5	12.5	74	14	707.3	69.6	0.463	-266.899	-321.075	-321.075	Ret C16	Ret C36	Ret C36 - F
19	2325.1	2335.2	19	157	32	700	68.1	1.214	-240.356	-296.494	-296.494	Ret C16	Ret C36	Ret C36 - F
20	2382.6	2389.5	15	149	32	693.8	66.1	0.852	-203.289	-262.166	-262.166	Ret C16	Ret C36	Ret C36 - F
21	2396.9	2413.7	24.7	425	82	699.6	68	3.282	-250.565	-305.949	-305.949	Ret C16	Ret C36	Ret C36 - F
22	3483.2	3492.6	31.8	385	60	661	62.1	11.245	-445.061	-486.071	-486.071	Ret C16	Ret C36	Ret C36 - F
23	3582.3	3598.4	32.2	381	60	655.7	60.9	11.18	-435.556	-477.268	-477.268	Ret C16	Ret C36	Ret C36 - F

Peak	Trial 1	Trial2	Average	St Dev
1	17.8	24	23.4	375
2	97.8	117	23.2	368
3	194.6	204.2	27.4	366
4	298	313.3	21.5	359
5*	839.3	851.7	26.1	1910
6	1608.9	1613.1	9.4	58
7	1648.4	1655.1	12.7	133
8	1853.6	1857.8	9.2	78
9	2037.1	2054.1	27.2	226
10	2138.5	2143.5	10.9	68
11	2152.5	2158.6	11.7	124
12	2164.2	2167.5	8.2	113
13	2177.6	2182.8	13	61
14	2262.8	2269.5	12.7	193
15	2275.6	2292.7	21.9	721
16	2297.5	2299.6	5.2	92
17	2302.8	2305.7	6.1	69
18	2308.8	2313.8	16.1	73
19	2324.9	2334.9	20.7	151
20	2380.5	2389.3	16.7	153
21	2396.7	2413.3	24.2	431
22	3483.2	3511.8	31.6	251
23	3581.8	3588.7	34.3	253

Peak	Trial 1	Trial2	Average	St Dev
1	-249.433	-285.571	-267.502	25.55342
2	-287.948	-287.122	-287.535	0.58407
3	-313.442	-257.657	-285.65	39.30453

Peak	Trial 1	Trial2
1	218	226
2	702	721
3	425	431

Peak	Trial 1	Trial2	Average	St Dev
1	-285.997	-321.541	-303.769	25.13301
2	-305.221	-303.954	-304.587	0.895602
3	-338.993	-283.177	-311.085	39.46807

Ret C16	Ret C36	Ret C36 - F	Ret unknow	Ret unk - F	Norm ret	Correction	Ass. Error
841.9	4033	3191.1	2054.3	1212.4	0.379932	-5.79966	-2.62859
841.9	4033	3191.1	2293.1	1451.2	0.454765	-8.94198	-3.03845
841.9	4033	3191.1	2413.7	1571.8	0.492557	-7.51889	-3.24544

Ret C16	Ret C36	Ret C36 - F	Ret unknow	Ret unk - F	Norm ret	Correction	Ass. Error
851.7	4033	3181.3	2054.1	1202.4	0.377959	-5.76954	-2.61778
851.7	4033	3181.3	2292.7	1441	0.452959	-8.91443	-3.02856
851.7	4033	3181.3	2413.3	1561.6	0.490899	-7.49311	-3.23619

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Peak number	Start time	Retention	Width	Amp2	Amp3	Backgrou	Backgrou	Area all	rD	3H2/2H2	d	3H2/2H2	d	2H/1H
1812 18ab #1														
1	17.8	23	24.2	247	39	660.7	62.5	4.771	-441.174	-482.472	-482.472			
2	99.3	105.5	22.2	245	38	661.5	62.6	4.665	-436.268	-477.928	-477.928			
3	198.6	208.4	21.7	241	38	664.2	62.3	4.622	-429.105	-471.294	-471.294			
4	297.6	306.8	22.6	234	38	663.2	62.4	4.496	-422.762	-465.419	-465.419			
5*	841.2	852.3	24.2	1850	430	673.5	64.2	9.168	0	-73.9	-73.9			
6	1482	1488.5	13.8	153	34	668.8	64.5	0.674	-211.893	-270.134	-270.134			
7	1576.1	1581.7	10.5	125	27	690.5	68.2	0.465	-171.44	-232.67	-232.67			
8	1665.7	1671.4	12.5	97	22	687.5	66.2	0.404	-174.797	-235.779	-235.779			
9	1710.9	1715.9	12.7	74	16	680.9	65.7	0.324	-238.238	-294.532	-294.532			
10	1738.5	1743.5	14.2	52	11	686.2	66	0.446	-139.476	-203.069	-203.069			
11	1752.7	1758.1	11.7	176	39	686.2	66	0.896	-191.163	-250.936	-250.936			
12	1836.3	1840.9	9.4	83	18	688.1	67	0.344	-205.003	-263.753	-263.753			
13	1902.3	1908.2	15	139	31	700.4	69.4	1.172	-184.576	-244.836	-244.836			
14	1917.4	1922.8	9.6	292	63	700.4	69.4	1.475	-202.923	-261.827	-261.827			
15	1927	1929.1	14.2	98	21	700.4	69.4	0.818	-198.688	-257.905	-257.905			
16	1994.7	2000.3	9.8	165	37	748.9	80.8	0.679	-191.229	-250.997	-250.997			
17	2057.4	2065.5	16.1	557	119	731.6	77.7	4.022	-221.976	-279.472	-279.472			
18	2073.5	2078.1	15	297	60	731.6	77.7	1.539	-287.117	-339.799	-339.799			
19	2122.8	2128.7	11.3	120	27	703.1	69	0.714	-151.044	-213.782	-213.782			
20	2134.1	2138.3	13	134	30	703.1	69	0.877	-182.987	-243.364	-243.364			
21	2147.1	2153.5	12.1	165	37	703.1	69	1.057	-198.918	-258.118	-258.118			
22	2159.2	2163.4	8.6	117	26	703.1	69	0.697	-207.381	-265.955	-265.955			
23	2167.7	2170.7	10	79	17	703.1	69	0.429	-158.899	-221.057	-221.057			
24	2179	2184.1	9.6	52	12	706.4	70.5	0.242	-168.468	-229.919	-229.919			
25	2188.6	2201	18.4	978	208	706.4	70.5	7.372	-223.641	-281.014	-281.014			
26	2207	2212.7	13.6	445	94	706.4	70.5	3.467	-231.034	-287.861	-287.861			
27	2220.6	2224	15	96	20	706.4	70.5	0.922	-237.404	-293.76	-293.76			
28	2235.7	2243	13.4	78	17	706.4	70.5	0.65	-192.713	-252.371	-252.371			
29	2249	2254.7	9.4	73	15	706.4	70.5	0.429	-214.931	-272.948	-272.948			
30	2258.5	2265.6	18	93	19	706.4	70.5	0.984	-217.012	-274.874	-274.874			
31	2276.4	2284.2	15.5	151	32	706.4	70.5	0.984	-227.936	-284.991	-284.991			
32	2305.9	2312.6	21.7	91	19	723.3	74	0.914	-241.42	-297.479	-297.479			
33	2338.5	2343.3	7.7	182	39	724.3	73.7	0.786	-199.585	-258.736	-258.736			
34	2346.2	2350	15.7	215	47	724.3	73.7	1.967	-214.822	-272.847	-272.847			
35	2383	2388.5	9.2	79	17	702.7	69.1	0.414	-187.108	-247.181	-247.181			
36	2462.4	2482.3	27.6	94	20	692.8	67	1.34	-230.097	-286.993	-286.993			
37	2596.8	2606.6	19.4	85	20	700.5	67.3	0.818	-101.496	-167.895	-167.895			
38	2678.8	2684.2	13.4	57	13	710.6	69.6	0.365	-120.854	-185.823	-185.823			
39	2724.5	2730.2	13.8	58	15	717.4	70.9	0.391	-66.699	-135.67	-135.67			
40	3483.4	3496.6	33.6	171	27	667.6	62.7	4.941	-427.143	-469.477	-469.477			
41	3583.1	3601.1	31.8	167	27	667.9	63	4.821	-422.944	-465.588	-465.588			
2229 18ab #2														
1	19.6	29.5	22.4	161	26	657.3	62.5	3.09	-407.688	-451.459	-451.459			
2	99.3	104.7	21.7	162	27	657.4	62.2	3.066	-402.154	-446.335	-446.335			
3	198.8	212.8	21.5	163	26	661.2	62.7	3.106	-422.291	-464.984	-464.984			
4	298.5	309.9	21.9	160	26	664	62.6	3.054	-405.153	-449.112	-449.112			
5*	840	852.9	26.1	2111	476	665.7	64.3	10.953	0	-73.9	-73.9			
6	1483.5	1488.5	13.8	150	33	674.2	64.8	0.644	-190.539	-250.358	-250.358			
7	1576.9	1581.7	11.1	122	27	688	68.3	0.463	-197.123	-256.455	-256.455			
8	1665.9	1671.8	12.1	97	21	680.4	65.7	0.397	-180.957	-241.484	-241.484			
9	1712.5	1716.3	10.4	72	15	678.8	65.6	0.292	-198.106	-257.366	-257.366			
10	1753.3	1758.1	10	147	32	709.1	71.9	0.533	-152.771	-215.381	-215.381			
11	1836.3	1841.5	9.6	86	18	686.5	67.1	0.358	-225.32	-282.569	-282.569			
12	1901.9	1908.4	15.3	131	30	696.5	68.5	1.149	-157.92	-220.15	-220.15			
13	1917.2	1922.8	10.5	293	63	696.5	68.5	1.536	-186.748	-246.847	-246.847			
14	1927.6	1929.5	8.4	93	20	696.5	68.5	0.596	-159.048	-221.194	-221.194			
15	1993.7	2001	11.1	161	36	743.8	80.4	0.694	-210.019	-268.399	-268.399			
16	2058	2066	15.7	524	114	739.5	78.4	3.829	-206.06	-264.732	-264.732			
17	2073.7	2078.5	16.1	276	58	739.5	78.4	1.412	-269.226	-323.231	-323.231			
18	2123.2	2128.9	11.3	124	26	702.8	68.8	0.74	-197.341	-256.658	-256.658			
19	2134.5	2138.5	9.4	131	29	702.8	68.8	0.766	-186.109	-246.256	-246.256			
20	2147.9	2153.3	11.5	147	31	725.9	74	0.791	-221.936	-279.435	-279.435			
21	2159.4	2163.8	8.6	100	21	725.9	74	0.532	-263.169	-317.621	-317.621			
22	2168	2170.9	10.9	56	11	725.9	74	0.242	-283.769	-336.698	-336.698			
23	2189.7	2201	17.8	943	201	715.6	71.7	7.097	-215.229	-273.224	-273.224			
24	2207.5	2213.3	13.4	427	91	715.6	71.7	3.201	-214.2	-272.271	-272.271			
25	2220.8	2224.6	9.8	84	19	715.6	71.7	0.592	-190.819	-250.617	-250.617			

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26	2262.8	2266.2	6.5	60	11	741.7	78.1	0.238	-303.282	-354.77	-354.77
27	2276.8	2284.2	15.3	118	25	735.8	76.3	0.509	-197.403	-256.715	-256.715
28	2306.1	2312.2	19.9	86	19	719.5	73.1	0.887	-201.749	-260.74	-260.74
29	2338.5	2343.1	7.7	168	37	721.5	73.9	0.728	-188.887	-248.829	-248.829
30	2346.2	2349.8	15.7	211	46	721.5	73.9	1.825	-215.513	-273.486	-273.486
31	2382.4	2388	9.4	82	17	696	69	0.357	-255.851	-310.844	-310.844
32	2463.5	2468.9	8.8	69	16	694.9	67.2	0.303	-128.43	-192.839	-192.839
33	2472.3	2482.3	18.6	88	20	694.9	67.2	0.876	-167.346	-228.879	-228.879
34	2595.8	2606.9	19.6	90	19	692.7	67.3	0.972	-220.278	-277.899	-277.899
35	2676.9	2684.2	16.9	56	13	704.4	68.6	0.462	-106.054	-172.117	-172.117
36	3483.6	3511	31.6	123	20	662.3	62.5	3.5	-417.825	-460.848	-460.848
37	3583.1	3604	32	120	20	665.1	62	3.368	-376.786	-422.842	-422.842
coinj G 0004											
1	19.4	38.2	21.7	733	123	321.4	88.7	14.356	-440.911	-482.228	-482.228
2	98	104.3	24.7	730	122	323.9	88.9	14.325	-439.416	-480.843	-480.843
3	197.7	213.2	23.2	731	123	322.8	88.8	14.417	-440.778	-482.106	-482.106
4	298.2	311.6	21.7	726	121	325.4	89.5	14.217	-441.84	-483.088	-483.088
5*	908.5	919.6	27	2644	639	330.1	90.3	14.235	0	-73.9	-73.9
6	1528.2	1534.9	19.9	751	180	336.9	91.1	3.088	-109.072	-174.911	-174.911
7	1549.1	1555.2	11.1	52	12	339.3	92	0.207	-215.671	-273.633	-273.633
8	1819.3	1824.2	9.2	51	12	341	92.5	0.21	-181.113	-241.629	-241.629
9	1973.8	1987.8	32	106	25	339.2	91.7	1.243	-174.728	-235.716	-235.716
10	2060.7	2066.2	9.8	60	14	357.7	96.5	0.284	-178.163	-238.897	-238.897
11	2121.6	2129.3	17.3	191	46	354.6	94.4	1.586	-168.561	-230.004	-230.004
12	2138.9	2143.1	14.2	116	27	354.6	94.4	0.724	-190.181	-250.027	-250.027
13	2213.1	2218.7	11.1	55	13	353.4	94.3	0.289	-170.413	-231.719	-231.719
14	2249	2264.7	22.6	413	93	346.3	93.1	2.872	-216.68	-274.567	-274.567
15	2271.6	2277.1	13.6	177	39	346.3	93.1	1.318	-236.646	-293.057	-293.057
16	2404.1	2415	23	82	19	351.4	93.7	1.042	-202.552	-261.483	-261.483
17	3482.6	3504.7	32.6	657	110	322.1	88.6	19.395	-440.579	-481.92	-481.92
18	3583.1	3589.4	31.8	654	109	320.3	88.6	19.367	-441.145	-482.445	-482.445
coinj G 0005											
1	19	30.7	22.2	645	107	322.1	89.2	12.608	-442.603	-483.795	-483.795
2	98.9	102.2	22.2	641	107	321.2	88.9	12.549	-440.175	-481.546	-481.546
3	198.6	203.1	22.4	639	106	320.6	88.6	12.574	-439.557	-480.974	-480.974
4	297.6	301.8	22.2	637	107	322.6	88.3	12.471	-436.572	-478.21	-478.21
5*	909.2	920.6	25.9	2813	672	327.2	89.8	15.532	0	-73.9	-73.9
6	1528.8	1535.5	17.1	758	181	336.2	90.1	3.093	-83.749	-151.46	-151.46
7	1551.4	1555.4	11.7	53	12	336.9	91.4	0.236	-170.39	-231.698	-231.698
8	1983.4	1988.2	18.2	85	20	362.7	98	0.449	-237.639	-293.978	-293.978
9	2061.4	2066.6	9.2	57	15	360.1	96.9	0.259	-136.271	-200.101	-200.101
10	2123.6	2129.9	15.3	204	47	353.7	95	1.584	-185.673	-245.852	-245.852
11	2138.9	2143.3	21.9	116	26	353.7	95	0.754	-264.778	-319.111	-319.111
12	2212.3	2219.2	12.5	60	14	349.9	94.1	0.337	-242.049	-298.061	-298.061
13	2254.1	2264.9	17.8	421	96	347.9	93.3	2.823	-208.856	-267.322	-267.322
14	2271.8	2277.5	14.2	178	40	347.9	93.3	1.341	-220.39	-278.003	-278.003
15	2404.8	2408.9	7.1	63	15	352.6	93.7	0.265	-145.841	-208.963	-208.963
16	2411.9	2415.6	15.3	81	19	352.6	93.7	0.755	-182.965	-243.344	-243.344
17	3482.8	3508.1	32.2	578	96	322.7	88.5	17.044	-438.702	-480.182	-480.182
18	3582.7	3596.1	32.4	575	95	323.9	89.1	17.013	-439.998	-481.383	-481.383
coinj G 0006											
1	19.4	23	21.7	564	94	322.8	89.2	11.028	-440.471	-481.82	-481.82
2	97.2	114.5	24.2	564	95	322.5	88.9	11.05	-438.586	-480.074	-480.074
3	198.3	211.3	22.6	561	93	326.9	89.9	11.027	-440.703	-482.035	-482.035
4	298.2	308.3	21.7	557	93	324	89.1	10.905	-437.695	-479.25	-479.25
5*	906.6	920.6	30.9	2843	679	326.8	89.9	15.907	0	-73.9	-73.9
6	1528.6	1535.7	21.3	873	205	332.3	91.3	3.728	-126.746	-191.279	-191.279
7	1550.6	1555.6	14.6	61	14	337.8	91.6	0.276	-172.109	-233.29	-233.29
8	1810.4	1824.8	19.2	70	17	334.9	90.9	0.496	-152.805	-215.413	-215.413
9	1968.8	1974.2	14.8	59	14	337.1	91.7	0.532	-200.057	-259.173	-259.173
10	1983.6	1988.4	23.6	136	31	337.1	91.7	1.155	-188.856	-248.799	-248.799
11	2062.2	2066.6	9.6	74	18	361.9	97.9	0.35	-176.956	-237.779	-237.779
12	2123.6	2130.3	15.5	237	56	359.2	96.3	1.832	-187.84	-247.859	-247.859
13	2139.1	2143.7	16.3	135	31	359.2	96.3	0.823	-216.78	-274.66	-274.66
14	2189.9	2203.7	23.4	66	15	344.9	92.1	0.783	-160.956	-222.961	-222.961
15	2213.3	2219.4	11.1	85	20	344.9	92.1	0.516	-173.829	-234.883	-234.883
16	2224.4	2229.2	9.2	58	13	344.9	92.1	0.372	-188.392	-248.37	-248.37

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17	2255.9	2265.4	16.1	484	112	357	94.5	3.267	-201.549	-260.555	-260.555
18	2272	2277.9	14.2	212	48	357	94.5	1.562	-202.006	-260.977	-260.977
19	2343.7	2349.8	14.6	52	11	362.8	96.4	0.215	-193.522	-253.121	-253.121
20	2405	2415.6	23	99	23	355.9	94	1.213	-156.077	-218.443	-218.443
21	3482.8	3493.2	33	508	85	321.7	88.6	14.968	-438.365	-479.869	-479.869
22	3581.6	3585.4	33.6	504	84	321.8	88.7	14.922	-438.114	-479.637	-479.637

Peak	Trial 1	Trial 2	Average	St Dev
1	-285.3273	-270.5873	-277.9573	10.42275
2	-287.5173	-279.7273	-283.6223	5.508362

Peak	Trial 1	Trial 2	Trial 3	Average	St C
1	-177.9713	-154.5205	-194.2958	-175.5959	20

Peak	Trial 1	Trial 2
1	557	524
2	978	943

Peak	Trial 1	Trial 2	Average	St Dev
1	-306.4164	-292.684	-299.5502	9.710309
2	-299.3194	-292.1306	-295.725	5.083237

18ac

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Peak number	Start time	Retention	Width	Amp2	Amp3	Backgroun	Backgroun	Area all	rD	3H2/2H1	d	3H2/2H2	d	2H/1H
18ac coinj G 0006														
1	19.4	28.2	21.7	498	82	322.2	89.3	9.742	-441.774	-483.027	-483.027			
2	99.1	106	21.7	498	83	320.9	88.7	9.732	-435.852	-477.543	-477.543			
3	198.6	208	23	494	83	321.8	89.2	9.722	-438.224	-479.739	-479.739			
4	297.4	308.5	23.2	491	82	324.8	89.5	9.606	-437.965	-479.5	-479.5			
5*	907.7	920.4	28.2	3018	725	327.2	89.9	17.6	0	-73.9	-73.9			
6	1527.4	1534.7	18.2	704	170	329.5	90.4	2.967	-108.17	-174.076	-174.076			
7	2286.7	2292.1	13.4	64	16	338.7	90.8	0.318	-72.1	-140.672	-140.672			
8	2445.9	2454.5	18.4	226	49	333	90	1.191	-211.315	-269.599	-269.599			
9	2464.3	2470.4	18.4	87	20	333	90	0.635	-230.326	-287.205	-287.205			
10	3483.4	3505.3	31.8	447	74	324.8	89.5	13.14	-435.383	-477.108	-477.108			
11	3581.2	3607.8	33.6	446	74	322.6	89	13.195	-433.649	-475.503	-475.503			

Peak number	Start time	Retention	Width	Amp2	Amp3	Backgroun	Backgroun	Area all	rD	3H2/2H1	d	3H2/2H2	d	2H/1H
18ac coinj G 0007														
1	18.8	25.9	22.8	439	74	318.3	88.5	8.602	-437.147	-478.742	-478.742			
2	98.4	116.6	23.2	438	73	321	89.1	8.557	-435.999	-477.679	-477.679			
3	198.6	208	21.9	434	73	323.3	89.3	8.532	-434.154	-475.97	-475.97			
4	298.2	307.2	21.7	435	72	321.2	89.2	8.507	-436.645	-478.277	-478.277			
5*	908.3	920.6	33.4	3093	757	326.1	90.1	18.719	0	-73.9	-73.9			
6	1527.2	1534.7	19.2	717	173	327.6	90.6	3.004	-106.17	-172.224	-172.224			
7	2285.8	2291.5	15.3	67	16	332.4	90.6	0.327	-95.199	-162.064	-162.064			
8	2444.5	2454.3	19.6	223	49	331.2	90.2	1.239	-199.9	-259.027	-259.027			
9	2464.1	2470.2	17.8	95	21	331.2	90.2	0.679	-227.235	-284.342	-284.342			
10	3483	3508.3	32	395	66	318.6	88.7	11.626	-433.398	-475.27	-475.27			
11	3582.9	3590.4	31.8	393	66	320	89.4	11.614	-435.535	-477.249	-477.249			

Peak	Trial 1	Trial 2	Trial 3	Average	St Dev
1	-177.138	-175.284		-176.211	1.311219

peak #2	start	ret	width	amp2	amp3	back 2	back 3	area all	rd	3h2/2h2	d	2h/1h
1	20.1	34.3	20.9	89	14	644.7	62.4	1.679	-444.001	-485.09	-485.09	
2	99.7	113.1	21.5	93	13	645.2	62.8	1.704	-469.005	-508.245	-508.245	
3	199.4	214.9	21.1	90	14	649	62.5	1.689	-445.212	-486.211	-486.211	
4	298.9	311.8	20.7	93	14	650.3	62.9	1.663	-451.741	-492.257	-492.257	
5*	842.7	854.8	23	2866	657	672.8	64.6	17.678	0	-73.9	-73.9	
6	2219.4	2226.1	16.7	224	48	698.2	67.6	1	-195.299	-254.767	-254.767	
7	2380.1	2394.7	21.3	535	105	691.2	66.3	4.037	-215.469	-273.446	-273.446	
8	2401.4	2410	20.9	306	61	691.2	66.3	1.951	-249.7	-305.147	-305.147	
9	3484	3489	30.5	80	12	645.6	62	2.196	-498.502	-535.562	-535.562	
10	3583.5	3588.7	31.4	78	11	646.5	62.5	2.183	-514.941	-550.787	-550.787	
#1												
1	19.9	23	21.1	119	19	652.8	62.5	2.238	-425.079	-467.566	-467.566	
2	99.5	101.8	21.5	117	19	650.7	62.1	2.218	-408.034	-451.78	-451.78	
3	199	209.2	23	116	20	655.2	61.6	2.241	-393.173	-438.017	-438.017	
4	297.6	304.5	21.9	110	19	664.3	62.9	2.024	-384.771	-430.237	-430.237	
5*	842.9	854.2	23	2497	570	669.7	64.1	14.492	0	-73.9	-73.9	
6	2220.8	2226.1	13.2	223	50	692.5	67.1	0.994	-154.165	-216.672	-216.672	
7	2379.3	2395.6	22.8	542	105	682.9	66.1	4.293	-221.176	-278.731	-278.731	
8	2402	2410.8	17.1	324	65	682.9	66.1	2.047	-254.813	-309.882	-309.882	
9	3484	3500.1	30.7	97	15	654.6	62.4	2.717	-455.922	-496.129	-496.129	
10	3583.5	3610.9	31.1	91	14	659	62.6	2.536	-424.779	-467.287	-467.287	

Peak	Trial 1	Trial 2	Avg	Stdev
1	-261.386	-223.291	-242.339	26.93762
2	-280.872	-286.161	-283.516	3.739757
3	-312.646	-317.385	-315.015	3.350513

Peak	Trial 1	Trial 2
1	224	223
2	535	542
3	306	324

Peak	Trial 1	Trial 2	Avg	Stdev
1	-297.503	-259.481	-278.492	26.88542
2	-302.626	-307.7	-305.163	3.588116
3	-343.617	-347.412	-345.515	2.68374

Peak number	Start time	Retention	Width	Amp2	Amp3	Backgrou	Backgrou	Area all	rD	3H2/2H:	d	3H2/2H2	d	2H/1H
19ab coinj G 0001														
1	19.4	20.7	21.7	1587	263	691.2	62.4	31.047	-430.5	-472.586	-472.586			
2	98.2	101.2	23	1580	261	685.1	61.7	30.953	-432.135	-474.1	-474.1			
3	198.6	215.1	21.9	1564	257	685.8	62.4	30.817	-434.042	-475.866	-475.866			
4	298.2	301.8	21.9	1550	255	689.7	62.1	30.351	-431.707	-473.704	-473.704			
5*	909.6	922.9	24.5	2982	677	692.9	61.6	19.505	0	-73.9	-73.9			
6	1404.1	1409.9	13.6	84	18	695.4	63.5	0.387	-288.275	-340.871	-340.871			
7	1527	1535.3	18.2	582	129	700	63.2	2.357	-104.407	-170.591	-170.591			
8	2213.1	2218.7	11.1	57	12	702.9	64	0.302	-201.638	-260.637	-260.637			
9	2254.3	2269.1	27.6	1124	224	712.9	66	8.092	-220.554	-278.155	-278.155			
10	2402.2	2407.7	8.4	94	20	712.1	65.8	0.423	-182.866	-243.252	-243.252			
11	2410.6	2413.9	13.4	120	25	712.1	65.8	0.855	-240.699	-296.811	-296.811			
12	2535.6	2540.8	9.2	124	28	709.6	65.2	0.575	-197.837	-257.117	-257.117			
13	2544.8	2545.8	7.7	58	11	709.6	65.2	0.239	-361.841	-409.001	-409.001			
14	2662	2667.5	13	88	21	705.4	62.9	0.537	-107.614	-173.561	-173.561			
15	3483.2	3507.6	33.2	1253	203	683.2	60.9	36.989	-435.964	-477.646	-477.646			
16	3581.2	3596.1	33.4	1240	201	683	60.8	36.749	-435.455	-477.175	-477.175			

Peak number	Start time	Retention	Width	Amp2	Amp3	Backgrou	Backgrou	Area all	rD	3H2/2H:	d	3H2/2H2	d	2H/1H
19ab coinj G 0002														
1	18.2	21.5	23.4	1205	194	684.4	61.7	23.598	-434.841	-476.606	-476.606			
2	98.4	114.7	22.8	1201	194	681.2	61.6	23.516	-435.411	-477.134	-477.134			
3	198.3	207.3	23.2	1195	192	680.9	61.9	23.559	-437.567	-479.131	-479.131			
4	298.2	311.4	21.5	1187	191	681.7	61.7	23.205	-436.1	-477.772	-477.772			
5*	909.4	922.7	27.2	3137	725	692.3	62.2	21.152	0	-73.9	-73.9			
6	1405.1	1409.1	11.1	104	22	698.5	63.6	0.41	-194.338	-253.877	-253.877			
7	1527.2	1534.9	17.3	668	147	698.8	63.2	2.779	-115.932	-181.265	-181.265			
8	2123.4	2130.5	12.5	58	13	707.9	64.1	0.373	-129.541	-193.868	-193.868			
9	2212.1	2218.3	11.5	70	15	703.8	64.2	0.412	-278.447	-331.769	-331.769			
10	2223.6	2227.9	9.2	58	11	703.8	64.2	0.369	-270.273	-324.199	-324.199			
11	2254.1	2269.1	27.4	1276	244	715.7	66.4	9.468	-219.102	-276.81	-276.81			
12	2401.8	2406.8	8.2	113	24	718.5	66.6	0.501	-216.455	-274.359	-274.359			
13	2410	2413.3	14.4	128	29	718.5	66.6	0.947	-222.408	-279.872	-279.872			
14	2534.8	2540.4	9	150	33	714.4	65.1	0.698	-186.479	-246.598	-246.598			
15	2543.7	2545.2	10.9	65	14	714.4	65.1	0.255	-178.408	-239.124	-239.124			
16	2659.3	2666.4	16.5	108	25	706.8	63	0.683	-120.692	-185.673	-185.673			
17	3483.2	3497.6	32.2	961	154	689.3	61	28.309	-434.785	-476.554	-476.554			
18	3582.9	3604.8	32.6	955	152	686.7	61.4	28.24	-437.782	-479.33	-479.33			

Peak number	Start time	Retention	Width	Amp2	Amp3	Backgrou	Backgrou	Area all	rD	3H2/2H:	d	3H2/2H2	d	2H/1H
183512 19ab #1														
1	18.8	32.6	22.4	1168	186	661.8	62.3	22.835	-446.808	-487.689	-487.689			
2	99.1	108.3	23	1170	186	661.2	62.3	22.899	-448.735	-489.474	-489.474			
3	198.3	204	22.2	1161	185	666.8	62.9	22.831	-448.524	-489.278	-489.278			
4	298.2	318.3	21.9	1154	184	669	63.1	22.589	-448.096	-488.882	-488.882			
5	367.2	377	20.7	187	41	658.5	62.5	2.221	-232.922	-289.609	-289.609			
6*	842.7	850.6	19	1213	286	668.1	63.8	5.102	0	-73.9	-73.9			
7	2188	2202.4	28.4	1140	227	702.1	68.9	8.125	-218.128	-275.908	-275.908			
8	2337	2348.5	22.8	119	25	690.5	67.5	1.425	-288.827	-341.382	-341.382			
9	2471	2476.2	8.6	119	26	693.8	66.3	0.546	-176.476	-237.334	-237.334			
10	2479.6	2481.5	9	52	12	693.8	66.3	0.23	-167.783	-229.284	-229.284			
11	2595.2	2602.7	19.4	93	21	683.8	64.5	0.678	-192.545	-252.216	-252.216			
12	3483.2	3497.8	31.8	1024	162	667.2	62.3	30.255	-450.997	-491.568	-491.568			
13	3581.6	3599.2	34.9	1019	161	666.1	61.9	30.192	-448.907	-489.633	-489.633			

Peak number	Start time	Retention	Width	Amp2	Amp3	Backgrou	Backgrou	Area all	rD	3H2/2H:	d	3H2/2H2	d	2H/1H
195623 19ab #2														
1	19.4	20.5	21.9	2514	426	661	62.8	49.27	-436.812	-478.432	-478.432			
2	98.6	100.1	24	2490	422	664.1	62.7	48.693	-435.465	-477.184	-477.184			
3	198.6	199.8	24.7	2443	415	669.4	62.9	48.944	-434.966	-476.722	-476.722			
4	297.8	299.3	22.4	2413	411	662.1	59.3	47.271	-430.205	-472.313	-472.313			
5*	842.7	850.6	18	1267	305	676.9	64.2	5.529	0	-73.9	-73.9			
6	2188.2	2200.4	24	791	159	691.4	66.3	4.559	-201.865	-260.848	-260.848			
7	2335.4	2348.3	24.7	61	13	689.1	65.9	0.794	-266.28	-320.502	-320.502			
8	2469.8	2474.8	9	61	14	690.9	65.2	0.287	-81.613	-149.482	-149.482			
9	3483	3492.6	32	1585	260	665.4	61.9	46.78	-437.416	-478.991	-478.991			
10	3582.7	3593.1	32	1562	256	665.1	62.5	46.266	-438.722	-480.201	-480.201			

Peak number	Start time	Retention	Width	Amp2	Amp3	Backgrou	Backgrou	Area all	rD	3H2/2H:	d	3H2/2H2	d	2H/1H
153941 19ab coinj G														
1	19	39.7	24.2	806	126	674.3	61.4	15.855	-435.966	-477.648	-477.648			
2	98.9	111.8	24.2	799	125	677.4	61.7	15.603	-435.495	-477.212	-477.212			
3	196.7	199.8	25.3	844	125	674.2	61.6	16.859	-440.062	-481.441	-481.441			
4	298.2	306	21.5	791	124	677	61.9	15.466	-439.689	-481.096	-481.096			
5*	800.3	811.8	24.7	1096	254	671.1	62.4	6.143	0	-73.9	-73.9			
6	1464.5	1469.9	15	83	20	684.8	63.5	0.384	-39.776	-110.737	-110.737			
7	2192.8	2198.9	14.6	189	42	689.8	62.9	0.904	-106.421	-172.457	-172.457			
8	3481.3	3492	36.2	651	102	670.3	61.3	19.183	-438.815	-480.287	-480.287			
9	3582.7	3608.6	31.8	649	100	667.7	61.7	18.984	-439.869	-481.263	-481.263			

Peak	Trial 1	Trial 2	Trial 3	Trial 4	Average	St Dev
1	-173.649	-184.2696			-178.9593	7.5099147

19ab CONT

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2 -284.7993 -283.418 -282.3922 -267.3226 -279.483 8.1667234

Peak	Trial 1	Trial 2	Trial 3	Trial 4
1	582	668		
2	1124	1276	1140	791

Peak	Trial 1	Trial 2	Trial 3	Trial 4	Average	St Dev
1	-194.0138	-202.3608			-198.1873	5.9022223
2	-294.3059	-290.8321	-291.6656	-282.6255	-289.8573	5.0434357

Peak number	Start time	Retention time	Width	Amp2	Amp3	Background	Background	Area all	rD 3H2/2H2	d 3H2/2H2	d 2H/1H
#2											
1	20.3	31.4	20.7	64	8	640.5	62.8	1.206	-585.253	-615.903	-615.903
2	99.9	111.8	20.7	68	8	638.7	62.5	1.267	-584.995	-615.664	-615.664
3	199.4	202.1	22.4	71	8	642.8	63	1.39	-630.151	-657.483	-657.483
4	299.1	302.4	21.1	72	8	643	63.1	1.335	-633.576	-660.655	-660.655
5*	842.3	852.7	22.8	2216	522	682.4	62.4	12.065	0	-73.9	-73.9
6	1853.2	1858.4	12.1	127	26	688.9	64.8	0.554	-215.959	-273.899	-273.899
7	2036.9	2049.5	20.3	129	27	690.7	65.9	0.893	-210.608	-268.944	-268.944
8	2319.7	2333.5	26.8	616	126	708.3	67	4.187	-179.797	-240.41	-240.41
9	2380.7	2388.5	15.7	169	35	704.3	67.4	0.856	-230.776	-287.621	-287.621
10	2398.7	2407.9	18.6	229	48	710.6	68.1	1.219	-175.638	-236.559	-236.559
11	2458.9	2468.1	12.5	90	20	699.1	66.4	0.432	-205.849	-264.537	-264.537
12	3484	3485.9	30.7	62	9	642.2	62.2	1.701	-609.534	-638.39	-638.39
13	3583.7	3604.8	32.6	64	7	638.1	62.6	1.846	-671.708	-695.969	-695.969
#1											
1	20.3	36.2	20.7	77	11	649.4	62.6	1.411	-493.887	-531.288	-531.288
2	99.9	104.9	20.5	75	10	645.8	62.6	1.386	-501.232	-538.091	-538.091
3	199.4	209.8	20.7	76	11	646.9	62.4	1.404	-489.459	-527.188	-527.188
4	298.9	312.7	20.7	74	11	648.8	62.7	1.361	-490.158	-527.835	-527.835
5*	843.1	857.7	32	3764	881	674.2	64.1	28.122	0	-73.9	-73.9
6	1852.8	1859.1	13.6	146	31	684	65	0.673	-224.536	-281.843	-281.843
7	2039	2051.1	19.6	146	30	697.7	66.9	1.075	-221.639	-279.16	-279.16
8	2220	2225.4	10	57	12	697.7	67.3	0.263	-153.977	-216.498	-216.498
9	2250.3	2255.3	11.3	56	12	715.5	71.3	0.211	-206.101	-264.77	-264.77
10	2320.3	2334.9	24	671	134	698.5	67.1	4.846	-179.965	-240.566	-240.566
11	2382.2	2389.5	17.1	190	40	704.1	67.8	0.991	-194.216	-253.764	-253.764
12	2399.3	2409.4	20.1	262	54	704.1	67.8	1.609	-207.999	-266.528	-266.528
13	2463.3	2469.1	9.2	112	23	703.1	67.5	0.505	-220.423	-278.033	-278.033
14	3484	3491.8	30.5	72	8	642.9	62.5	1.963	-591.362	-621.56	-621.56
15	3583.7	3613.2	31.6	72	9	645	62.2	2.042	-578.904	-610.023	-610.023

Peak	Trial 1	Trial 2	Avg	Stdev
1	-247.544224	-247.704884	-247.624554	0.113604096

Peak	Trial 1	Trial 2
1	616	671

Peak	Trial 1	Trial 2	Avg	Stdev
1	-266.97236	-265.722135	-266.347248	0.884042221

25ac

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Peak number	Start time	Retention	Width	Amp2	Amp3	Backgroun	Backgroun	Area all	rD	3H2/2H: d	3H2/2H2	d 2H/1H
27ac #1												
1	19.4	33.6	21.7	925	153	263.4	92.5	18.133	-450.016	-490.659	-490.659	
2	98.4	103	22.4	924	153	263.4	92.2	18.111	-447.507	-488.336	-488.336	
3	198.1	208.2	22.4	921	153	262.1	91.9	18.16	-447.367	-488.206	-488.206	
4	297.2	311.2	23.6	920	152	261.6	92.1	18.04	-448.223	-488.999	-488.999	
5	584.4	601.7	34.9	103	30	268.8	93.8	1.72	64.805	-13.884	-13.884	
6*	911.7	926.3	30.7	3980	978	270	94.9	27.965	0	-73.9	-73.9	
7	1527.8	1537.2	20.5	376	91	278.4	97	1.442	-113.057	-178.602	-178.602	
8	1554.8	1562.3	10.2	115	27	280.2	96.8	0.474	-141.843	-205.261	-205.261	
9	1565	1568.8	15.5	212	43	280.2	96.8	0.89	-262.147	-316.674	-316.674	
10	1899.8	1914.9	24.5	556	114	281.4	97.2	3.237	-209.393	-267.819	-267.819	Ret C16
11	1924.3	1932	17.3	329	70	281.4	97.2	1.626	-238.199	-294.496	-294.496	911.7
12	2067.2	2078.7	24	239	61	294.7	100.5	1.314	-159.412	-221.532	-221.532	911.7
13	2104.6	2120.9	19.6	192	42	302.2	101.5	1.381	-195.453	-254.909	-254.909	911.7
14	2124.3	2131.2	19.2	161	38	302.2	101.5	1.661	-171.157	-232.408	-232.408	911.7
15	2143.5	2148.5	15.7	62	16	302.2	101.5	0.494	-160.007	-222.082	-222.082	
16	2257.8	2264.9	14.6	89	21	329.3	108	0.442	-192.767	-252.421	-252.421	
17	2361.7	2369	14.4	61	15	335.5	109.1	0.335	-178.465	-239.176	-239.176	
18	2391	2400.2	13.4	348	79	325.6	107	1.869	-179.072	-239.739	-239.739	
19	2404.3	2407.7	16.1	133	29	325.6	107	0.795	-252.201	-307.463	-307.463	
20	2451.8	2480.2	32.4	1459	287	343	111	20.994	-255.7	-310.704	-310.704	
21	2484.2	2494.4	22.2	848	164	343	111	6.678	-293.194	-345.427	-345.427	
22	2570.3	2581.1	32.2	78	15	398.5	125.4	0.848	-616.958	-645.264	-645.264	
23	2793.1	2840.5	87.8	262	62	353.8	113.5	9.334	-192.45	-252.128	-252.128	
24	3091.1	3144	75	269	57	314.3	104.2	8.152	-199.54	-258.694	-258.694	
25	3483.6	3489.3	33	884	147	253.4	91.3	26.096	-447.24	-488.089	-488.089	
26	3581.8	3592.1	33	880	145	252.4	91.7	26.103	-449.616	-490.289	-490.289	
27ac #2												
1	19.4	37.6	21.9	871	144	253.1	91.5	17.052	-449.074	-489.787	-489.787	
2	99.1	108.5	21.7	869	143	254	92.2	17.015	-451.249	-491.802	-491.802	
3	198.6	209	22.6	867	143	253.4	91.8	17.102	-449.924	-490.575	-490.575	
4	298.2	301.8	23.4	865	143	253	91.5	16.97	-448.786	-489.52	-489.52	
5*	908.7	924	32.4	3965	973	259.3	93.4	27.575	0	-73.9	-73.9	
6	1529.5	1534.7	13.6	326	80	266.3	95.1	1.237	-113.539	-179.049	-179.049	
7	1554.3	1559.6	7.9	101	23	267.9	95.1	0.375	-158.772	-220.939	-220.939	
8	1562.3	1566.2	13.6	195	40	267.9	95.1	0.827	-240.967	-297.06	-297.06	
9	1899.4	1911.7	22.4	485	100	266.4	94.6	2.684	-222.406	-279.87	-279.87	Ret C16
10	1921.8	1928.7	17.8	286	61	266.4	94.6	1.376	-248.127	-303.69	-303.69	908.7
11	2064.9	2075.4	21.1	150	38	277.5	96.4	0.78	-99.902	-166.42	-166.42	908.7
12	2104	2115.1	16.1	110	24	282.1	97.6	0.708	-208.463	-266.958	-266.958	908.7
13	2120.1	2127.6	21.7	87	21	282.1	97.6	0.96	-160.227	-222.287	-222.287	908.7
14	2385.5	2394.9	14	192	44	294.5	100.3	0.927	-185.982	-246.138	-246.138	
15	2399.5	2402.9	11.5	70	15	294.5	100.3	0.378	-241.123	-297.204	-297.204	
16	2445.5	2469.3	28.6	1016	198	300.6	101.6	10.972	-249.489	-304.952	-304.952	
17	2474.1	2482.9	28.2	527	105	300.6	101.6	3.636	-301.385	-353.013	-353.013	
18	2819.4	2855.1	65.2	152	28	377	123	4.243	-440.151	-481.524	-481.524	
19	3483.2	3485.7	33	831	137	249.9	91.6	24.548	-449.808	-490.467	-490.467	
20	3582.9	3590.2	32	827	136	249.7	91.6	24.522	-451.149	-491.709	-491.709	
27ac #3												
1	19.4	34.9	21.7	819	135	250.1	91.2	16.052	-449.069	-489.783	-489.783	
2	99.1	116.8	21.9	818	134	249.8	91.3	16.018	-450.973	-491.546	-491.546	
3	198.6	209	21.9	815	134	251.4	91.7	16.078	-451.153	-491.713	-491.713	
4	298.2	313.3	22.6	812	133	252.4	91.7	15.923	-449.723	-490.389	-490.389	
5*	907.9	924	33	4121	1013	256.2	93	29.13	0	-73.9	-73.9	
6	1529	1534.7	15.9	370	91	266.5	94.5	1.407	-95.612	-162.446	-162.446	
7	1553.9	1559.6	8.4	112	26	266.1	94.6	0.43	-165.112	-226.81	-226.81	
8	1562.3	1566.5	11.7	212	43	266.1	94.6	0.92	-241.057	-297.143	-297.143	
9	1898.1	1912.1	23.6	530	109	266.6	94.2	3.015	-211.168	-269.463	-269.463	Ret C16
10	1921.8	1929.1	20.3	315	65	266.6	94.2	1.601	-248.564	-304.095	-304.095	907.9
11	2065.8	2075.4	21.5	165	41	278.9	97.1	0.849	-146.032	-209.14	-209.14	907.9
12	2101.3	2115.1	18.4	120	26	282.3	97.7	0.78	-220.234	-277.858	-277.858	907.9
13	2119.7	2127.2	21.7	97	23	282.3	97.7	1.082	-184.935	-245.168	-245.168	907.9
14	2386.2	2394.5	12.7	212	49	293.9	99.7	1.036	-174.602	-235.599	-235.599	
15	2398.9	2402.2	16.7	77	18	293.9	99.7	0.46	-226.118	-283.308	-283.308	
16	2445.1	2469.5	29.1	1077	211	302.3	101.8	12.121	-249.194	-304.678	-304.678	
17	2474.1	2483.3	26.5	568	112	302.3	101.8	3.961	-297.199	-349.136	-349.136	
18	3483.4	3491.6	32	779	128	247.3	90.8	23.002	-451.559	-492.089	-492.089	
19	3583.1	3595.4	31.8	774	127	247.1	90.8	22.946	-452.831	-493.267	-493.267	

Peak	Trial 1	Trial 2	Trial 3	Average	St dev
1	-272.7252	-284.7706	-274.3682	-277.288	6.5319535
2	-299.4843	-308.672	-309.0816	-305.746	5.4266504
3	-318.37	-312.572	-312.301	-314.4143	3.4283672
4	-353.1599	-360.697	-356.8239	-356.8936	3.7690293

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Peak	Trial 1	Trial 2	Trial 3
1	556	485	530
2	329	286	315
3	1459	1016	1077
4	848	527	568

Peak	Trial 1	Trial 2	Trial 3	Average	St dev
1	-293.844	-308.1432	-296.277	-299.4214	7.650615
2	-329.2593	-340.7578	-339.5741	-336.5304	6.3246758
3	-323.5732	-323.7452	-322.5123	-323.2769	0.6677415
4	-367.3149	-382.6995	-377.5904	-375.8683	7.8355073

LETTER-TO-NUMBER KEY

1	A
2	B
3	C
4	D
5	E
6	G
7	H
8	I
9	J
10	K
11	L
12	M
13	N
14	O1
15	O2
16	P
17	Q
18	R
19	S
20	B'
22	D'
23	E'
24	F'
25	G'
26	H'bulk
27	H'lean
28	H'rich
29	I'
30	F wood 006
31	F wood 019
32	F wood 025
33/34	F wood 038
35	F wood 044
36	F paleosol 008
37	F paleosol 006
38	F paleosol 007
39	G' layer amber
40	B' layer amber
41	M layer amber
42	Mixed amber