**IN-PROCESS DETECTION OF WELD DEFECTS USING LASER-BASED
ULTRASONIC LAMB WAVES**

Stephen W. Kercel
Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831

Marvin B. Klein and Bruno Pouet
Lasson Technologies, 6059 Bristol Parkway, Culver City, CA 90230

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ABSTRACT

Laser-based ultrasonic (LBU) measurement shows great promise for on-line monitoring of weld quality in tailor-welded blanks. Tailor-welded blanks are steel blanks made from plates of differing thickness and/or properties butt-welded together; they are used in automobile manufacturing to produce body, frame, and closure panels. LBU uses a pulsed laser to generate the ultrasound and a continuous wave (CW) laser interferometer to detect the ultrasound at the point of interrogation to perform ultrasonic inspection. LBU enables in-process measurements since there is no sensor contact or near-contact with the workpiece.

The authors have used laser-generated plate (Lamb) waves to propagate from one plate into the weld nugget as a means of detecting defects. This report recounts an investigation of a number of inspection architectures based on processing of signals from selected plate waves, which are either reflected from or transmitted through the weld zone. Bayesian parameter estimation and wavelet analysis (both continuous and discrete) have shown that the LBU time-series signal is readily separable into components that provide distinguishing features, which describe weld quality. The authors anticipate that, in an on-line industrial application, these measurements can be implemented just downstream from the weld cell. Then the weld quality data can be fed back to control critical weld parameters or alert the operator of a problem requiring maintenance. Internal weld defects and deviations from the desired surface profile can then be corrected before defective parts are produced.

The major conclusions of this study are as follows. Bayesian parameter estimation is able to separate entangled Lamb wave modes. Pattern recognition algorithms applied to Lamb mode features have produced robust features for distinguishing between several types of weld defects. In other words, the information is present in the output of the laser ultrasonic hardware, and it is feasible to extract it. Wavelet analysis produces results that are almost as good as Bayesian, but execute a thousand times faster. This study demonstrates the principle that it is feasible to construct a laser ultrasonic system to detect weld defects in thin metal parts on-line in real-time, and to classify the defects according to type.

Keywords: "laser-based ultrasonic," "weld inspection," "on-line inspection," "Bayesian," and "wavelet."

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1. INTRODUCTION

The automotive industry is continually re-engineering its manufacturing processes to effect cost savings, enhance quality, reduce weight, and improve safety. One new process with all these attributes is associated with the fabrication of sheet metal panels for auto body manufacture. Different areas of the body have varying requirements for strength and corrosion resistance. Older manufacturing techniques either used single panels of sheet metal with stiffeners and protective coatings, or multiple panels with the proper characteristics which were attached separately to the body frame. In a new design-for-manufacturing approach, manufacturers are now producing large sheet metal panels or blanks made from smaller, individually engineered panels that are butt-welded together using a CO₂ or Nd:YAG laser welding process. With this approach, panels with differing thickness, metallurgy, or surface treatment can be joined to provide the desired attribute only in positions where it is required. Compared to conventional methods, the advantages of these tailor-welded sheet metal blanks are:

- less tooling and better integration of parts,
- forming with a single set of dies,
- reduction in manufacturing steps and in part count,
- superior dimensional control,
- reduction in overall weight,
- improved crash energy management,
- corrosion resistance, higher strength only where required,
- lower net cost, and
- better fit during assembly, resulting in less body noise.

In the United States, the production of tailor-welded blanks for 1997 is estimated to be 8 million blanks worth approximately \$25 million and made from 110,000 tons of sheet steel. The corresponding measure of welds produced is on the order of 10 miles per day. This production rate is expected to increase by a factor of 10 by the turn of the century.

In the blank welding process, the adjacent edges of the two panels to be welded are held at a fixed gap or in contact and the panels are then advanced under the stationary laser fixture. The most critical weld condition that must be controlled is the integrity and shape of the weld nugget formed between adjacent base metal surfaces. The desired transition from one surface to the other is smooth and flat, as shown in Figure 1. Either a concave or a convex surface is a sign of a lower strength weld. Typically, a concave surface can arise from poor fit-up or seam tracking, incomplete weld penetration or excessive weld penetration. Additionally, any crack or lack of fusion is a weld defect.

Figure 1. Schematic Drawing of Normal Laser Butt Weld and Defective Welds.

On-line monitoring of weld quality is a crucial unsolved problem in the manufacture of tailor-welded blanks. The goal is to be able to detect the full range of defects that may be present. At the current time, process monitors (e.g., weld speed, laser current) have been implemented, and control of these parameters to maintain the desired weld quality has been attempted. However, these open-loop controls are not sufficiently effective. A closed loop control scheme is required, as shown in Figure 2. However, conventional sensing technology does not provide a suitable transducer.

Figure 2. Weld-Joint Sensor As Transducer In Closed-Loop Control Scheme.

Several acoustic, optical, and ultrasonic sensors have been studied. Acoustic emission from the weld process (measured with an external microphone) was found to be noisy and not a full measure of weld quality. Optical sensors based on measurement of the spectral emission from the weld plasma or fusion zone have been investigated. Some correlation with weld quality has been observed, but the discrimination is not strong. Finally, ultrasonic inspection using electromechanical acoustic transducers (EMAT) has been studied, and has been shown to be unable to detect all the flaws.

It is clear that the need remains to implement a sensor that could directly measure the nugget integrity and surface profile, and thus determine the strength of the weld. One approach is to measure the deflection angle of a laser beam reflected from the nugget surface. Such an approach has been attempted, but poor surface quality has prevented reliable measurement of the surface profile. In addition, both sides of the blank would have to be interrogated. In the absence of any reliable automated sensor, welded blanks in the factory are now inspected by visual means on a statistical basis. Destructive sectioning with micrographic examination is sometimes used to augment the visual inspection. If defective welds are found then the output from the most or the entire shift must be inspected and the welder must be recalibrated. Clearly, this approach leads to added cost in energy, materials, and labor. As an alternative to this *reactive* welder maintenance approach, it would be desirable to develop a sensor that would monitor the desired weld property directly and allow *proactive* intervention to correct the weld process in real time or to alert the operator that maintenance is required.

2. LASER ULTRASONICS

A technology that shows great promise for on-line measurement of weld quality in tailor-welded blanks is laser-based ultrasound (LBU). LBU is a technique for performing ultrasonic inspection using a pulsed laser to generate the ultrasound and a separate CW laser interferometer to detect the ultrasound at the point of interrogation. [1] Laser-based ultrasound has several significant advantages for this application. No sensor contact (or near-contact) with the workpiece is required, thereby allowing in-process measurements in the harsh welder environment (i.e., high temperatures, turbulent atmospheric environment, vibrating parts with rapid lateral motion). Both free-space and fiber-based delivery of optical energy can be implemented.

The authors are investigating the use of laser-generated plate (Lamb) waves propagating from one plate into the weld nugget as a means of determining the surface profile. The investigation is considering a number of inspection architectures based on processing of signals from selected plate waves, which are either reflected from, or transmitted through the weld zone. One goal is to identify the simplest generation technique, wave mode, wave propagation geometry, feature extraction process, and pattern recognition algorithm that will provide effective identification of defective welds. It is anticipated that these measurements can be implemented just downstream from the weld cell (see Figure 3), so that weld quality data can be fed back to control critical weld parameters (or alert the operator of a problem requiring maintenance). Any deviation or defects from the desired surface profile can then be corrected before defective parts are produced.

Figure 3. Schematic Diagram of Weld Inspection Geometry Using Transmitted Lamb Waves.

Recent advances in optical receiver technology can overcome some of the disadvantages of conventional laser-ultrasonic methods. [1] Adaptive interferometric receivers under development at Lasson allow the processing of speckled signal beams that result from the interrogation of machined surfaces. In conventional interferometric receivers, speckle is a source of phase error that can greatly reduce the receiver signal-to-noise ratio. In conventional LBU technology, multiple speckles can be avoided by focusing tightly to a single speckle, but this approach has the risk of signal "dropouts" due to the presence of "dark speckles." The other major advantage of the new adaptive receivers is that they are insensitive to noise at lower frequencies caused by workpiece vibration and by welder-induced turbulence in the path of the receiver probe laser.

One challenge in implementing LBU for process control is the relatively low signal-to-noise ratio. This problem could be overcome by using more sophisticated signal processing for LBU than has been used in the past. [2] The signals produced by the LBU receiver are non-stationary transients in the time-domain, and real-time wavelet analysis should lead to the most efficient method of feature extraction. Furthermore, embedded wavelet processes are implementable in real-time hardware, and are effective for many pattern recognition problems for transient signals in severe noise. [3,4,5]

3. SIGNAL OVERLAP

One of the major problems in the analysis of signals from ultrasonic sensors is the fact that the signal of interest is often overlapped with many other signals [6]. The feature of interest (such as a localized weld defect) produces a signal that contains desired information (such as the distance of the weld defect from the point of ultrasonic excitation). However, other features (such as the edges of the workpiece) also produce signals that overlap the signal of interest, but contain no relevant information. In addition, the signals are inherently non-stationary, and equally inseparable in the time domain and the Fourier frequency domain. Finally, the signal of interest may be considerably weaker than the obscuring signals.

The key to the signal-processing problem is to separate the desired signal from the undesired signals while not destroying the desired information with the process. To appreciate the idea, consider a sensor signal that is the sum of four overlapping Gabor functions plus a low-level Gaussian-distributed random function. Also consider that the information of interest is contained in one of the Gabor functions. (Note: A Gabor function is a Gaussian-windowed sinusoid. Its waveform is completely characterized by four parameters, the frequency and phase of the sinusoid, and the peak location and width of the window.)

In this example, suppose that each of the Gabor functions is produced by a different physical feature, and that we can tell something about the feature (for example, its location in space) by examining the parameters of the Gabor function associated with that specific feature. The problem is that we must disentangle the underlying Gabor functions given the overlapped signal. As shown in Figure 4, the signal is the sum of a low level of Gaussian noise and four Gabor functions, with normalized frequencies of 0.025, 0.05, 0.025, and 0.05, and window peaks at time delays of 600, 1400, 1400, and 600 respectively. The components are not conveniently separable in either the time or frequency domains.

Figure 4. Signal Overlapped in Time and Frequency.

Suppose we have prior knowledge from our understanding of the underlying physical process that the signal should contain one or more Gabor functions, but we have no prior knowledge of the parameters such as frequency or the time of the window peak. By the methods of Bayesian parameter estimation [7], we can use the Gabor function as a model, and guess a frequency and a time. We can project the signal shown in Figure 4 onto the model, and compute the log likelihood that the Gabor function with the guessed parameters fits the data. If we repeatedly guess sets of parameter values, and plot the resulting log likelihoods against the guessed parameter values, we obtain the plot shown in Figure 5.

Another way of saying this is that Figure 5 is the projection into log likelihood space of the signal shown in Figure 4. When we examine this composite signal in log likelihood space, we see four well-separated components, and expect that we should be able to recover each component, one by one. The two parameters are, ω , the oscillation frequency (0-0.06) and τ , the time of occurrence (0-2000) of the event. The vertical dimension is the log-likelihood that the observed data contains a Gabor function with the given pair of the parameter values.

Figure 5. Likelihood of Fit of Signal to Gabor Function.

Given the signal shown in Figure 4, the most likely Gabor function that fits the signal, is the one whose parameters lead to the greatest log likelihood. Using a global optimizing algorithm, with the objective function being the log likelihood as a function of the time and frequency parameters, we can readily find the optimal combination of parameters. (Note that local optimization algorithms such as gradient descent are vulnerable to being trapped in local optima.) As indicated by the peak in Figure 4, the optimum value of the objective function occurs at a time of 605.4 and a frequency of 0.0248.

The most likely Gabor function in the signal shown in Figure 4 is plotted in the left-hand plot in Figure 6. This is the Gabor function whose parameters are found at the global optimum in Figure 5. When this estimated signal is subtracted from the signal in Figure 4, the residual in the right-hand plot of Figure 6 is obtained. Note that the most likely Gabor function has been separated from the signal without disturbing the other information in the signal.

Figure 6. Most Likely Signal and Residual.

Since we have reason to believe that the signal should contain several Gabor functions plus noise, we can apply precisely the same methods to the residual, and obtain the next most likely signal, and its residual with the next likeliest Gabor function removed. In Figure 7 we see the results of repeating this process until the residual is reduced to noise. The second through fourth likeliest Gabor functions have times of 1397.9, 612.2 and 1400.9 and frequencies of 0.0251, 0.050, and 0.050 respectively. The residual after removing the four likeliest Gabor functions is noise and cumulative rounding error.

Figure 7. Other Components of Overlapped Signal.

The point of the foregoing discussion is to demonstrate that overlapping signals can be separated without disturbing each other. Bayesian parameter estimation provides the optimal estimates of the models underlying the signal, however it is computationally costly. For the purposes of on-line real-time monitoring, the goal is to find a method that is almost as good as Bayesian, but much faster.

In laser ultrasonic, the signals of interest are oscillating bursts. This suggests that wavelet analysis might produce acceptable performance for an on-line instrument. The wavelet basis function is an oscillating burst, and the discrete wavelet transform is implemented as a bank of computationally inexpensive finite impulse response (FIR) digital filters.

The idea behind wavelet analysis is that the signal can be considered as the weighted sum of overlapping wavelet functions [8]. In fact, any signal of finite bandwidth and finite duration can be completely characterized as a weighted sum of a finite number of scaled and shifted versions of the underlying wavelet. The concept is similar to Fourier analysis, in which the time series signal can be considered a weighted sum of sinusoids at various frequencies, with the transform

coefficients being the weights. The practical meaning of the wavelet transform of a signal is that each coefficient of the transform is the weight, or relative amount of information that the wavelet at that particular value of scale and shift contributes to the overall signal.

For the results reported in the next section, the wavelet analysis was performed with the Daubechies 10-coefficient least asymmetric discrete wavelet. [9] Discrete wavelets are not expressible in closed form. Plots of the wavelet and its corresponding scaling function were computed with Daubechies cascade algorithm, and are shown in Figure 8.

Figure 8. Wavelet and Scaling Functions for 10-Coefficient Least Asymmetric Wavelet.

Suppose that a time-domain input consists of a list of 960 evenly spaced samples of a band-limited signal. The discrete wavelet analysis results in a list of 960 wavelet-domain coefficients output in response to each 960-element time series input signal. As sinusoids at different frequencies are orthogonal to each other, so also are scaled and translated versions of these wavelet functions orthogonal to each other. This means that Parseval's theorem holds for discrete wavelet transform; the amount of energy in the signal in the wavelet domain is exactly the same as the amount of energy in the signal in time domain. Energy is regarded as proportional to the information in the signal.

For a transient signal, such as an oscillating burst, it is expected that most of the energy in the signal will be concentrated in relatively few of the wavelet coefficients, with all the others having values very close to zero. The energy contributed by each coefficient is the square of the coefficient. The fraction of the total signal energy contributed by each coefficient is the energy of the coefficient divided by the total energy of the signal (the sum of the squares of all the samples of either the time series or all the wavelet coefficients). Sorting the wavelet coefficients from greatest to smallest, the cumulative energy of each coefficient is the fraction of total signal energy contributed by that coefficient, plus the fractions of signal energy contributed by all the larger coefficients. For a typical data set collected in this research, the largest coefficient (out of 960) contains over 30% of the total energy of the signal, and that the ten largest contain over 98% of the total signal energy.

The discrete wavelet packet transform is a generalization of the discrete wavelet transform. As shown in Figure 9, each stage of both the wavelet transform and the wavelet packet transform consists of an elemental pair of filters (high-pass and low-pass) that splits the input signal into two decimated orthogonal components. The low-pass output is an approximation of the input signal. The high-pass output contains the details of the input signal that are missing from the approximation. There is no information in the two outputs that overlaps, and nothing is lost. The input signal can be exactly reconstructed from the two outputs.

Figure 9. Elemental Filter Pair.

The discrete wavelet transform is implemented by cascading the elemental filter pairs as shown in Figure 10, and the wavelet packet is implemented by cascading them as shown in Figure 11. In the wavelet transform configuration, the low-pass output of the preceding stage is fed into an identical copy of the elemental filter pair. Thus the first approximation is further approximated, and the second set of details consists of the information present in the first approximation but absent from the second. In wavelet parlance, the output of the first high-pass filter is the set of wavelet transform coefficients of the input signal at the finest scale. The output of the next high-pass filter is the set of wavelet transform coefficients of the input signal at the next finer scale. The output of the final low-pass filter is the set of scaling function coefficients. The cascade can be repeated as often as necessary, and all the outputs are orthogonal.

There is no fundamental reason why the high-pass output of the elemental filter pair cannot be split as well, and nothing to prevent repeating this process as often as necessary. A filter bank in which at least some of the high-pass outputs are split into other approximations and details implements the wavelet packet transform [10]. If the high-pass output is split whenever the low-pass output is split, then the system is a complete wavelet packet transform. However, it is not necessary for the wavelet packet to be complete. A more efficient representation of the signal may be obtained by leaving out some of the filter pairs in the cascade. Irrespective of how many filter pairs are included, all outputs are orthogonal.

For any given input signal, there is an optimal configuration of filter pairs that represents most of the input signal energy with the fewest coefficients. This is known as the best basis wavelet packet. The best basis is determined by finding the configuration of filter pairs whose output has the highest entropy [11].

Energy is regarded as proportional to the information in the signal. Suppose that a signal's energy consists of three major elements. In addition to the energy of the desired signal, there may be coherent or non-random signals produced as undesired, but unavoidable biasing artifacts due to the hardware. Also, there may be broadband high-frequency energy that is typically regarded as random noise. If these three energies are separable in wavelet space, then the undesired bias and noise components of the sensor output signal can be identified and subtracted from the original sensor output. What remains is the signal of interest with its features unobscured.

Figure 10. Implementation of The Discrete Wavelet Transform.

The reason for transforming a time-series into another domain is to try to find a more compact representation of the information in the data. The performance of the different transforms can be compared by considering how effectively each compresses the same data set. The rationale for using data compression for the first step in pattern recognition feature selection is that it is more effective to search for features in a short list of numbers than a long list.

Figure 11. Implementation Of The Wavelet Packet Transform.

The effectiveness of several transforms was compared by taking the same list of 960 numbers (generated by a laser ultrasonic sensor), and producing an output list of 960 numbers. In each output list, there are relatively few big numbers, and relatively many numbers close to zero. The idea is that the useful information is in the few big numbers, and that the many small ones can be zeroed out without much loss of the underlying information. This is the conceptual basis for data compression.

The wavelet packet, the discrete wavelet, and the discrete Fourier transform are all orthogonal. Since Parseval's theorem holds, the energy in the output data set is identical to the energy in the input data set. For each transform output data set, the cumulative energy function counts up the cumulative energy in the output coefficients as energy is accumulated by counting energies, starting from the energy of the greatest transform coefficient, and moving to the smallest [12]. In the following example, we compute the normalized cumulative energy of the wavelet packet transform, the discrete wavelet transform, and the discrete Fourier transform of the same signal from a laser ultrasonic sensor.

In the upper left of Figure 12, as the plot of the first 200 members of the cumulative energy list shows, for the output of the best basis wavelet packet transform, virtually all of the information is contained in the biggest 135 members. The other 825 members are very close to zero. The upper right of Figure 5 shows the cumulative energy for the discrete wavelet transform, using the same input signal, and the same elemental filter pair (Daubechies least asymmetric 10-coefficient filter and its paraunitary companion). The lower left of Figure 12 is for the Fourier transform; it

is clearly far less effective than the other two at compressing the signal. The lower right shows all three cumulative energies overlaid. The best basis wavelet packet transform is only marginally superior to the wavelet transform for this data set, and not worth the added cost compared to the wavelet transform.

Figure 12. Cumulative Energy of The Same Signal In Different Transform Spaces.

In many cases, once the signature of interest is separated from everything else in the sensor signal, the detection of flaws in the workpiece is straightforward. Typically, the workpiece is scanned across a physical range by the LBU apparatus. Continuity of the mathematical properties of the signature across scans suggests an unflawed workpiece. The appearance of an abrupt discontinuity, such as a dramatic localized change in peak of window location (often suggesting a localized change in time of flight of an ultrasonic echo) suggests the presence of a flaw.

Consistent interpretation of weld signatures must be model-based, where the model is in some reasonable sense a description of the underlying physical reality. The various bursts that appear in the sensor output have physical causes, and in ultrasonics, the physics of the causes is typically well understood. Signal processing by the methods described in this section exploit this knowledge to wring the maximum of new and relevant information from the sensor output data, and provide an indication of confidence in the results. This is in contrast with the widely popular paradigm of signal processing in which an empirical model is surmised without respect to the underlying process. The empirical approach works for some data sets, but give no indication of when it might break down for the next unknown trial.

4. PRELIMINARY RESULTS - BAYESIAN

A typical result of LBU inspection of a tailor-welded blank is shown in Figure 13. Each plot is the output voltage of a LBU photo-detector as a function of time, as the LBU system makes 30 successive scans across a workpiece with a flawed weld. It would be very difficult to detect the flaw simply from a visual inspection of these raw data.

From the data for each of the 30 scans, the most likely model (or dominant component) was computed using Bayesian parameter estimation. For each scan, the waveform of the most probable model is a chirped Gaussian-windowed sinusoid. The most probable is taken to be the dominant component of the signal. These are plotted in Figure 14. This dominant component appears to be a biasing effect characterizing the experimental setup. As shown in Table 1, this component contains approximately 95% of the signal energy for each scan.

The second likeliest component for the data of each of the 30 scans is plotted in Figure 15. For each scan, the first residual is computed by subtracting the estimated data for the likeliest component from the original data for the scan. The most probable model of the residual computed by Bayesian parameter estimation is taken as the second likeliest component of the original signal. For each scan, the waveform of the second likeliest component is a non-chirped exponentially rising sinusoid. This appears to be a reflection of an exponentially decaying sinusoidal component off the back of the workpiece. As shown in Table 1, the second likeliest component contains approximately 2-3% of the signal energy for each scan.

Figure 13. Successive Scans Across a Flawed Weld.

Figure 14. Likeliest Component of Each Scan.

Figure 15. Second Likeliest Component of Each Scan.

Figure 16. Third Likeliest Component of Each Scan.

Table 1. Percentage of Energy in Three Likeliest Components of Each Scan

Scan	1st	2nd	3rd	Scan	1st	2nd	3rd	Scan	1st	2nd	3rd
1	94.6	3.4	0.2	11	95.1	3.	0.2	21	96.	2.3	0.2
2	94.8	3.2	0.2	12	95.4	2.7	0.2	22	96.3	1.9	0.2
3	94.5	3.5	0.2	13	96.2	2.1	0.1	23	96.1	2.	0.1
4	94.9	3.2	0.2	14	95.6	2.5	0.1	24	95.8	2.	0.6
5	94.7	3.4	0.2	15	96.4	2.1	0.1	25	95.6	2.	0.9
6	95.3	2.8	0.1	16	95.7	2.5	0.2	26	96.4	2.	0.2
7	95.3	2.8	0.1	17	96.6	2.	0.1	27	95.8	2.3	1.6
8	95.3	2.8	0.1	18	96.	2.3	0.1	28	94.9	2.7	0.3
9	95.2	3.1	0.2	19	96.3	2.1	0.2	29	95.4	2.3	1.7
10	95.1	3.1	0.2	20	96.3	2.1	0.2	30	95.7	2.3	1.6

The third likeliest component for the data of each of the 30 scans is plotted in Figure 16. For each scan, the second residual is computed by subtracting the estimated data for the second likeliest component from the first residual for the scan. The most probable model of the second residual computed by Bayesian parameter estimation is taken as the third likeliest component of the original signal. For each scan, the waveform of the third likeliest component is the sum of several Gaussian pulses. This appears to be a reflection off the weld. As shown in Table 1, the third likeliest component typically contains less than 1% of the signal energy for each scan.

Figure 16 reveals some interesting information about the workpiece. For the first 21 scans, the third likeliest component is located consistently (except for scans 14 and 15) in the neighborhood of time = 500. This is consistent with a visually detectable pinhole flaw in the weld in the vicinity of scan 14. The inconsistent location of the third likeliest component in scans 22 through 30 suggests other flaws in the workpiece that are not revealed by visual inspection.

5. PRELIMINARY RESULTS – DISCRETE WAVELETS

The Bayesian parameter estimation algorithm has the disadvantage of comparatively high computational complexity. For an on-line real-time system, it is desirable to find an algorithm that gives performance that is almost as good as Bayesian, but with substantially lower computational cost. For example, discrete wavelet processing is almost as good as Bayesian for detecting short bursts and, being about three orders of magnitude faster than Bayesian, is fast enough to be implemented on a presently available digital signal-processing chip. For a given setup, the real-time algorithm might be wavelet-based, and the Bayesian analysis might be performed only occasionally, to verify calibration or to provide other guidance on how to exploit the wavelet output.

For these data, the tendency of the signal energy to concentrate in relatively few wavelet basis functions is shown in Table 2. Discrete wavelet transforms were computed of each of the 30 scans, using the 10-coefficient Daubechies least-asymmetric wavelet. For the first scan, the 8 largest wavelet coefficients contain 97% of the signal energy. The reason for asking which wavelet coefficients contain 97% of the signal energy is that the Bayesian analysis suggests that 97% of the signal energy is concentrated in the two likeliest components of the signal, and that these two components do not contain information about the weld. If we can find a cheap method of identifying this part of the signal, we can discard it with reasonable expectation that we are not discarding very much of the useful information in the signal. For the same scan, the 52 largest wavelet coefficients contain 99.99% of the signal energy. As shown in Table 1, other scans show a similar, but not identical energy distribution.

Table 2. Percentage of Energy in Largest Wavelet Basis Functions of Each Scan

Scan	97%	99.99%	Scan	97%	99.99%	Scan	97%	99.99%
1	8	52	11	7	60	21	7	61
2	8	58	12	7	68	22	7	57
3	8	53	13	7	62	23	7	66
4	7	56	14	8	54	24	8	51
5	8	62	15	7	63	25	8	62
6	7	49	16	7	53	26	8	69
7	7	49	17	7	54	27	8	60
8	7	49	18	7	51	28	8	61
9	7	56	19	7	62	29	8	57
10	7	53	20	7	58	30	8	65

This energy distribution is consistent with what was gleaned from the Bayesian analysis and provides a convenient way to parse the signal to eliminate irrelevant information. The largest 7 or 8 wavelet coefficients contain the 97% of the signal energy that does not include information about the weld. The largest 60 (or thereabouts) wavelet coefficients contain in excess of 99.99% of the total signal energy. This suggests that we can zero out the other 900 smallest and the 7 or 8 largest wavelet coefficients in each signal with practically no loss of information. The information that we seek resides in the part of the signal that remains.

Figure 17a was constructed as follows. The wavelet transform was computed for each signal. In wavelet space, the largest coefficients containing the first 99.99% of the signal energies were retained, and the others zeroed out. Then each zeroed-out set was inverse wavelet transformed to recover the approximate time series. Then each time series was subtracted from the corresponding original time series. The resulting residuals are plotted below as a density plot. The vertical axis corresponds to the 30 spatial locations on the workpiece. The horizontal axis corresponds to time. The gray level is strength. The residuals are mostly (but not entirely) noise.

In wavelet space, the 8 largest coefficients (containing 95-96% of the signal energies) were retained, and the others zeroed out. Then each zeroed-out set was inverse wavelet transformed to recover the approximate time series. Then each time series was subtracted from the corresponding original time series. The resulting 4-5% residuals are contour-plotted below in Figure 17b.

In the same wavelet space, the 9 largest coefficients (containing 96-97% of the signal energies) were retained, and the others zeroed out. Then each zeroed-out set was inverse wavelet transformed to recover the approximate time series. Then each time series was subtracted from the corresponding original time series. The resulting 3-4% residuals are contour-plotted in Figure 17c. Note that there is a little difference between Figure 17b and Figure 17c.

The reasonable place to search for features of weld defects is in the region of the signal between the bias (biggest eight coefficients of each signal, or thereabouts) and the noise (smallest 900

coefficients of each signal). In Figure 17d, 97.6% of the signal energy is assumed to be attributed to biasing effects. This bias is subtracted from the signal approximation constructed from the wavelet coefficients constituting of 97.8%, of the signal energy. This difference constitutes 1.2% of the original signal energy, and has a fairly dramatic global minimum whose contour is plotted in Figure 17d. This shows up in scan 14, and time 750. This corresponds to the change in the third likeliest component of the signal as revealed by Bayesian analysis, and to the pinhole defect in the weld in the workpiece.

Figure 17. Separation of Signal Energies by Wavelets.

It is noteworthy that a similar strategy of wavelet-based feature extraction was independently discovered by Legendre, *et al.* [13]. Their problem was the extraction of Lamb wave features from EMAT data. Their fundamental strategy was, as ours is here, to use the concepts developed by Donoho [14] to subtract out irrelevant features in both the fine and coarse scales of a discrete wavelet space, so that the residual would be dominated by flaw features. Their pattern recognition strategy differs from ours in that they used the recovered flaw features to obtain an image, while we use the data in the residual to obtain a numerical feature vector.

The compression effect is also the basis for Donoho denoising. Donoho says that for a wavelet transform of a noisy signal, the big coefficients hold the information and the small coefficients hold the noise. Since the wavelet compresses the information, a signal spread out in the time domain will be very compactly represented in the wavelet domain. On the other hand, noise is approximately evenly randomly distributed throughout both the wavelet and the time domains. The problem with Donoho's technique is that it is a bit of an art to decide where to draw the line between big coefficients and small ones.

Suppose we try to denoise with the best basis wavelet packet, by declaring that the biggest coefficients holding 90% of the total energy of the signal constitute the "information." In the left-hand plot of Figure 18, the jagged line is the original time series. The smooth line is constructed by taking the wavelet packet transform and identifying and retaining the 9 coefficients that hold 90% of the energy in transform space, and zeroing-out the 951 coefficients that contain the other 10% of the energy. The "denoised" time series is recovered by taking the inverse wavelet packet transform of the zeroed-out list. It is noted that the high frequency features of the time domain signal are mostly preserved (unlike the more traditional method of denoising by low-pass filtering), and noise is substantially reduced. However, it appears that there is some information being lost when we discard that last 10% of the energy.

A similar analysis was done by taking the wavelet packet transform and identifying and retaining the 35 coefficients that hold 98% of the energy in transform space, and zeroing-out the 925 coefficients that contain the other 2% of the energy. The "denoised" time series is recovered by taking the inverse wavelet packet transform of the zeroed-out list. In going from 90% to 98% of the signal energy (using the next 26 wavelet packet coefficients) it does not look at first glance that the next 26 coefficients bought us much.

The signal shown in Figure 18 is the 22nd of a set of 26 time series collected for a particular specimen.

Figure 18. Denoising a Laser Ultrasonic Signal.

6. THE OBSERVED EFFECT OF WELD FLAWS ON LAMB WAVE MODES

The utility of a commercial weld flaw detector depends on its ability to consistently detect the signatures of different weld types. Earlier research on this project showed that entangled Lamb wave modes could be readily separated by Bayesian parameter estimation. The objective of the latter part of the research in this project has been to investigate the effect of specific weld flaws on the mode structure in the expectation that a specific mode structures can be associated with specific types of weld flaws.

In early 2000, Lasson Technologies collected the sample 11 and sample 15 data sets in their laboratory. Sample 11 is a Tailor-welded blank with a good weld with low porosity. Sample 15 is a tailor-welded blank that is known to have high porosity from X-ray data.

For both samples, the Lamb waves were generated by firing an excitation laser through line-focused optics at the thin part of the sample. The receive optics used a point detection beam on the thick part of the sample. The spacing between generation and detection beams was about 42mm. The weld was between the detection and generation beams.

For both samples, what is actually being studied is the effect of the weld on the Lamb wave as it passes through the weld on a straight-line path from the excitation line to the receiving spot. To

observe the variation along the weld, the excitation and receive optics are scanned along the weld. In practice the scanning is done by holding the optics fixed, and moving the sample along the axis of the weld between successive scans. For sample 11, waveforms were collected for 55 scans. For sample 15, waveforms were collected for 52 scans. The samples were moved by 0.5mm between scans.

The model of each Lamb wave mode is assumed to be a Gaussian-windowed chirped sinusoid of the form

$$Ae^{\left(\frac{t-\tau}{\sigma}\right)^2} \cos \left[\alpha (t-\tau)^2 - (t-\tau) \omega \right] + Be^{\left(\frac{t-\tau}{\sigma}\right)^2} \sin \left[\alpha (t-\tau)^2 - (t-\tau) \omega \right]$$

where

t = the independent variable, and the parameters are

A and B = the amplitudes of the two components

τ = pulse group delay

σ = pulse width

ω = center frequency of oscillation

α = chirp rate

Each mode consists of a wave of this kind with a different set of values for the parameters.

For each scan of both samples, the parameters were estimated for the most likely modes. For each mode, the log likelihood (LL) is taken as a figure of merit. The greater the LL, the more likely the mode is present. For each mode, the “% erg” is the energy in the mode divided by the total energy of the signal. The results of the Bayesian analysis are tabulated in Appendix A.

The more pressing issue is, do all these numbers actually convey any meaning? To appreciate what they tell us about the process, consider the following. Figure 19 is a plot of sample 15 scan

Figure 19. Sample 15–Scan 1.

1. Blue is the raw data with the DC bias subtracted out. Red is the mode 1 component, obtained from Bayesian parameter estimation. The plots show signal intensity versus time.

For reliable pattern recognition, the relevant question is, do any of the parameters tend to cluster in an isolated region of parameter space? In particular, are the clusters well separated by class? What is desired in this case is a parameter value that is distinctly different for the class of high-porosity welds, and the class of good welds.

In these observations, the fifth likeliest mode showed the strongest tendency to form distinct clusters. The fifth mode for the good welds tend to look very similar to each other. The fifth mode for the high-porosity welds tend to look very similar to each other. However, the fifth modes for the two classes tend not to look like each other.

Figure 20 is a plot of the Gaussian Distributions based on the means and standard deviations of the dominant frequency of mode 5. Blue is Sample 15. Red is sample 11. The frequencies of mode 5 tend to cluster, but the cluster for sample 11 does not appear to be especially well separated from the cluster for sample 15.

Figure 20. Distribution of Frequencies in Mode 5.

Can we improve the classification by exploiting coincidence between these two parameters? If both the concentrations of energy in mode 1 (Figure 21) and the frequencies in mode 5 are caused by the difference in porosity of the samples, then we would expect there to be an exploitable coincidence between the two features. If mode 1 has a high concentration of energy, AND mode 5 has a low frequency, then it is much more likely that the signature is that of a high-porosity weld than that of a good weld.

Figure 21. Distribution of % Energies in Mode 1.

Suppose that each scan of each sample is characterized by a feature vector or ordered pair consisting of the frequency of mode 5 and the % energy of mode 1. Figure 22 is the plot of the ordered pairs for both samples. Red is sample 15. Blue is sample 11. Horizontal axis is frequency of mode 5. Vertical axis is % energy in mode 1. A possible decision criterion would be that we could detect high porosity if we consider all the scans of a sample and observe if there were any scans with % energy in mode 1 above 78%, AND with frequency of mode 5 below 0.035 radians/sec.

Figure 22. Weld Features In 2D Feature Space.

The quartile ellipses show the comparative compactness (or lack thereof) of the clusters. They are centered on the centroids of the sample lists for each class. The innermost ellipse encloses 25% of the samples of the class. The middle ellipse encloses 50% of the samples of the class. The innermost ellipse encloses 75% of the samples of the class. In Figure 23, we see the quartile ellipses superimposed over the 2D features. Notice that the 75th percentile ellipse for each class is outside the 75th percentile ellipse for the other. Thus, we are reasonably well separated. If we found yet another coincident parameter in the data, we could probably improve the separation of the classes further.

Figure 23. Quartile Ellipses for the Two Classes in Feature Space.

The concept illustrated by the quartile ellipses is equivalent to the idea of Mahalanobis distance. Suppose that x is an n -dimensional feature vector, and that a given class is defined by a cluster of n -dimensional feature vectors, whose mean (or centroid) is μ , and whose covariance matrix is cv . The Mahalanobis distance from sample x to the cluster is given by the following formula.

$$\text{mahalanobis} = \sqrt{(\mathbf{x} - \boldsymbol{\mu}) \cdot \text{Inverse}[\mathbf{cv}] \cdot (\mathbf{x} - \boldsymbol{\mu})}$$

The practical meaning of the Mahalanobis distance is as follows. The location of the cluster center is its centroid. Any given sample of the cluster has some probability of being a member of the cluster. The surfaces of constant probability are given by a family of hyper-ellipsoids centered on the centroid. The eigenvectors of the covariance matrix of the cluster point in the directions of the axes of the hyper-ellipsoid. The ratios of the lengths of the eigenvectors are the same as the ratios of the lengths of the axes of the hyper-ellipsoid. Thus, the covariance matrix and centroid define the location, orientation, and shape of the entire family. The Mahalanobis radius is the single parameter that defines the size of the surface of constant probability, or the distance from the cluster center.

7. CONCLUSIONS AND FURTHER RESEARCH

The authors have detected various kinds of weld flaws in various specimens of tailor-welded blanks using the methods described in this paper. These results demonstrate capability to detect localized weld defects using a computationally efficient processing approach that can be implemented in real-time at the frequencies at which these signatures occur. In ongoing research we are identifying the connection between the Bayesian-derived models and the underlying physical processes. We will also investigate the comparative reliability and computational cost of wavelet and Bayesian feature extraction methods.

In future work we will seek to classify individual defects, including those encountered in the welding process. We will also devise a practical implementation of the signal-processing algorithm in real time. The ultimate goal of this research is to construct a prototype of an on-line LBU weld inspection device for tailor-welded blanks.

This work could lead to spin-offs for other on-line inspection in other processes. Additional follow-on research might include the examination of other types of continuous seam joints for distinguishing features. In addition, the Lamb-wave modeling and feature extraction would be directly applicable to inspection of other products fabricated from thin metal sheet.

Bayesian parameter estimation is able to separate entangled Lamb wave modes. Pattern recognition algorithms applied to Lamb mode features have produced robust features for distinguishing between several types of weld defects. In other words, the information is present in the output of the laser ultrasonic hardware, and it is feasible to extract it. Wavelet analysis produces results that are almost as good as Bayesian, but execute a thousand times faster. This study demonstrates the principle that it is feasible to construct a laser ultrasonic system to detect weld defects in thin metal parts on-line in real-time, and to classify the defects according to type.

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APPENDIX A. RESULTS OF BAYESIAN ANALYSIS

For Sample 11 the Bayesian results consists of 1100 lines 10 features per line. The 10 features are : the sample name (S), the scan or trial number (T), the mode number (M), the log likelihood (LL) of the fit of the model to the data (greater magnitude => better fit), the radian frequency ($\omega = \pi$ radians/sec $\leftrightarrow$ frequency = 50 MHz), the window width (σ) in time bins (10 ns binwidth), the time of occurrence (τ) of the peak of the envelope in time bins, the chirp rate (α) in radians/sec/ sec, the fraction (% erg) of the total energy of the signal in this scan that is contained in this mode, and the phase angle (ϕ) in radians of this mode. ϕ is determined from the ratio of the amplitudes of the two components of the model.

Sample 11 Scan 1:

S	T	M	LL	w	s	t	a	% erg	f
S 11	1	1	891.486	0.0219528	241.34	1057.11	0.0000636014	0.589954	-0.582861
S 11	1	2	218.674	0.00705987	556.862	1610.6	-2.37292 ' 10 ⁻⁶	0.080417	-0.566525
S 11	1	3	257.457	0.0863169	77.3859	850.281	0.000121015	0.0746554	1.84485
S 11	1	4	143.665	0.164946	424.604	1088.97	-0.000028916	0.0340235	2.1575
S 11	1	5	62.6546	0.0592876	195.868	591.243	2.8123 ' 10 ⁻⁷	0.0133745	0.605648
S 11	1	6	109.317	0.0988647	196.927	1000.	-1.93821 ' 10 ⁻⁶	0.0177399	-2.05683
S 11	1	7	112.632	0.190437	199.158	800.	-3.0547545711078545 ' 10 ⁻⁹	0.0147756	0.906881
S 11	1	8	88.4211	0.169883	228.483	834.159	-6.95433 ' 10 ⁻⁶	0.0147299	-0.258868
S 11	1	9	48.8999	0.0879672	790.291	1292.13	-7.37616 ' 10 ⁻⁷	0.00761673	1.58724
S 11	1	10	127.659	0.207937	242.366	900.27	3.13609 ' 10 ⁻⁶	0.0181705	1.04786
S 11	1	11	142.289	0.114265	251.368	1000.	5.43806 ' 10 ⁻⁷	0.0112763	-0.709451
S 11	1	12	170.002	0.313122	136.598	1000.01	-2.4176 ' 10 ⁻⁷	0.0128465	-0.792714
S 11	1	13	210.183	0.136972	226.101	900.	3.1360449020868083 ' 10 ⁻⁶	0.0116638	0.167548
S 11	1	14	72.9812	0.0225386	591.298	922.174	7.5567287681535435 ' 10 ⁻⁶	0.00689933	-1.78984
S 11	1	15	168.348	0.274278	108.632	900.	8.22862 ' 10 ⁻⁶	0.0100348	0.0536383
S 11	1	16	97.8568	0.0476629	503.066	1154.97	-0.000019033	0.00755959	-1.05251
S 11	1	17	178.805	0.234476	98.4364	1200.	2.88116 ' 10 ⁻⁶	0.0115066	1.78805
S 11	1	18	87.0257	0.19791	313.6	1413.97	-0.000020744	0.00516971	-3.03261
S 11	1	19	90.9517	0.200192	882.212	2007.85	-0.000126249	0.00494305	-2.07839
S 11	1	20	90.7236	0.155374	182.522	1100.	3.1441697047851137 ' 10 ⁻⁶	0.00279217	2.4714

Sample 11 Scan 2:

S	T	M	LL	w	s	t	a	% erg	f
S 11	2	1	875.162	0.0222129	239.834	1054.73	0.0000639627	0.583206	-0.547991
S 11	2	2	206.9	0.00704514	554.066	1605.91	-2.3222365993759063 ' 10 ⁻⁶	0.0777925	-0.543461
S 11	2	3	163.619	0.0854657	225.631	904.618	-8.07172 ' 10 ⁻⁶	0.0370696	-2.2369
S 11	2	4	204.923	0.106506	221.458	1099.79	0.	0.0374659	0.546041
S 11	2	5	103.584	0.0666278	337.586	728.358	-0.0000130975	0.0259576	-2.02303
S 11	2	6	152.904	0.165477	422.429	1096.91	-0.0000285018	0.0337228	0.816999
S 11	2	7	81.1464	0.190468	209.481	799.977	-6.01935 ' 10 ⁻⁹	0.0157097	0.930013
S 11	2	8	79.226	0.0999091	551.028	1196.74	-6.78192 ' 10 ⁻⁶	0.0143507	-0.961162
S 11	2	9	89.0345	0.171874	247.926	899.873	-2.5722346843080974 ' 10 ⁻⁶	0.0148067	1.00869
S 11	2	10	123.398	0.207953	235.974	900.	3.5947655858951914 ' 10 ⁻¹⁰	0.017996	1.13307
S 11	2	11	185.191	0.136287	189.845	900.016	1.6388883613977106 ' 10 ⁻⁷	0.0159408	0.223874
S 11	2	12	175.676	0.3135	138.884	1000.	2.26329 ' 10 ⁻⁶	0.0135246	-0.792616
S 11	2	13	68.2568	0.048885	518.678	1043.38	8.6271 ' 10 ⁻⁷	0.0073757	-2.60597
S 11	2	14	75.9162	0.109453	348.893	895.46	-7.7246 ' 10 ⁻⁶	0.00763316	2.9412
S 11	2	15	76.5547	0.0235208	376.343	903.712	0.0000112768	0.00713239	-1.60665
S 11	2	16	222.467	0.274391	169.895	900.	5.14194 ' 10 ⁻⁶	0.0104972	0.0753802
S 11	2	17	172.393	0.234833	102.468	1200.	-1.1723828379304497 ' 10 ⁻⁶	0.0121616	1.74657
S 11	2	18	85.5987	0.198417	456.314	1405.92	-0.0000207564	0.0054955	-1.41224
S 11	2	19	77.6799	0.157631	307.009	1016.59	-5.46622 ' 10 ⁻⁶	0.00459589	2.83812
S 11	2	20	90.9174	0.0281614	342.053	1448.88	0.0000195685	0.00494468	1.84

Sample 11 Scan 3:

S	T	M	LL	w	s	t	a	% erg	f
S 11	3	1	864.81	0.0224522	239.674	1053.09	0.0000641533	0.578868	-0.517153
S 11	3	2	197.916	0.00704393	552.938	1603.96	-2.37346' 10 ⁻⁶	0.0755154	-0.528665
S 11	3	3	479.738	0.0850278	100.118	838.617	-5.69346' 10 ⁻⁶	0.0709824	3.05567
S 11	3	4	131.825	0.165495	425.186	1097.52	-0.0000285818	0.0338351	0.723567
S 11	3	5	176.899	0.108066	112.682	1100.	1.6267855233153072' 10 ⁻⁷	0.0323898	0.306036
S 11	3	6	120.065	0.190349	207.893	800.003	6.36962' 10 ⁻⁶	0.016377	0.850507
S 11	3	7	136.653	0.20762	224.963	900.	0.	0.0206027	1.12449
S 11	3	8	90.917	0.169575	229.227	836.227	-7.1273151877059466' 10 ⁻⁶	0.0148312	-0.6037
S 11	3	9	105.804	0.137045	240.042	900.	-5.09148' 10 ⁻⁶	0.0155157	0.186899
S 11	3	10	99.1462	0.0649509	131.696	579.109	-8.4597' 10 ⁻⁶	0.0121572	1.26583
S 11	3	11	178.749	0.313707	130.845	1000.	-2.0810252131660294' 10 ⁻⁶	0.0137742	-0.754415
S 11	3	12	68.7003	0.02272	549.2	919.225	8.10274' 10 ⁻⁶	0.00760025	-1.79851
S 11	3	13	170.528	0.274324	168.443	900.	3.1298460828493087' 10 ⁻⁶	0.0104969	0.141136
S 11	3	14	98.2679	0.0476843	423.717	1142.91	-0.0000169463	0.00902017	-0.485038
S 11	3	15	165.447	0.23459	97.6394	1199.77	5.07431' 10 ⁻⁶	0.0128109	1.77158
S 11	3	16	84.592	0.0939662	544.693	1244.11	0.0000161451	0.00604652	-0.349719
S 11	3	17	80.6218	0.198137	316.251	1424.83	-0.0000215143	0.00530568	1.10376
S 11	3	18	78.7497	0.107685	731.723	1553.74	0.0000300183	0.00478547	-0.250127
S 11	3	19	25.7424	0.219367	1264.24	1526.96	-5.89181' 10 ⁻⁷	0.00148433	1.57728
S 11	3	20	77.4835	0.0323452	544.689	1436.73	0.0000352199	0.00424398	2.10169

Sample 11 Scan 4:

S	T	M	LL	w	s	t	a	% erg	f
S 11	4	1	857.548	0.0225088	239.46	1052.24	0.0000644838	0.575799	-0.51437
S 11	4	2	191.966	0.00703487	555.122	1603.39	-2.30384' 10 ⁻⁶	0.0739968	-0.539556
S 11	4	3	177.168	0.0854821	227.508	916.826	-9.04888' 10 ⁻⁶	0.0381969	3.02942
S 11	4	4	140.598	0.10644	238.094	1100.	-9.53644' 10 ⁻⁶	0.0405613	0.665223
S 11	4	5	102.594	0.066616	344.263	729.536	-0.0000132051	0.0264054	-2.09559
S 11	4	6	143.887	0.165463	428.121	1098.04	-0.0000288724	0.0327532	0.638555
S 11	4	7	334.856	0.190439	54.2622	900.	4.73309' 10 ⁻⁷	0.0520551	0.870199
S 11	4	8	80.0995	0.100243	557.888	1193.79	-6.87373230340321575' 10 ⁻⁶	0.0122847	-0.650511
S 11	4	9	162.087	0.314124	128.245	1000.	-3.9369919032095197' 10 ⁻⁷	0.014816	-0.796789
S 11	4	10	58.5482	0.0488076	530.035	1037.62	1.0110043728356002' 10 ⁻⁶	0.00753444	-2.36476
S 11	4	11	126.257	0.237273	72.015	1200.47	8.21642' 10 ⁻⁶	0.0144941	1.41994
S 11	4	12	115.51	0.275336	129.698	900.016	-1.19995' 10 ⁻⁶	0.010485	0.181963
S 11	4	13	260.035	0.135425	233.107	900.	-1.0801015488809754' 10 ⁻⁷	0.0123995	0.0870388
S 11	4	14	87.9354	0.0235515	376.509	903.719	0.0000113115	0.00737237	-1.62832
S 11	4	15	128.79	0.111152	433.496	958.338	-9.17377' 10 ⁻⁶	0.00969228	2.4465
S 11	4	16	89.7403	0.200056	155.482	1393.34	-6.71476' 10 ⁻⁷	0.003968	0.759614
S 11	4	17	76.7992	0.158693	343.945	940.04	2.7027359092610103' 10 ⁻⁶	0.00491936	2.71102
S 11	4	18	61.5777	0.0590678	501.956	1458.76	6.27631' 10 ⁻⁶	0.00368035	1.20527
S 11	4	19	85.5809	0.0282582	353.688	1445.54	0.0000194648	0.00475282	1.91305
S 11	4	20	87.6795	0.0875979	349.538	1618.48	-0.0000177358	0.00446521	-1.39696

Sample 11 Scan 5:

S	T	M	LL	w	s	t	a	% erg	f
S 11	5	1	832.125	0.0262325	226.278	1028.02	0.0000634167	0.564876	0.0678032
S 11	5	2	189.779	0.00703124	518.721	1597.28	-1.9425739240131583' 10 ⁻⁶	0.0750616	-0.53149
S 11	5	3	191.991	0.0757899	329.841	854.54	-0.0000307704	0.0626997	2.02061
S 11	5	4	227.634	0.102225	242.024	907.563	-0.0000312083	0.0595752	2.44534
S 11	5	5	259.046	0.16616	254.72	1000.	1.2233799670839637' 10 ⁻⁶	0.0296011	-2.70935
S 11	5	6	308.122	0.190686	30.2898	901.787	0.000949068	0.0549049	0.16896
S 11	5	7	105.552	0.237107	278.483	1100.66	-5.83531' 10 ⁻⁶	0.0152406	0.300076
S 11	5	8	73.5581	0.0160453	166.817	1172.61	0.000116791	0.00970909	-1.53181
S 11	5	9	51.5803	0.109111	793.068	1143.51	-2.2586243034754917' 10 ⁻⁶	0.00639246	1.57783
S 11	5	10	88.6614	0.206284	230.638	1100.	-7.3966' 10 ⁻⁷	0.00618964	-2.51432
S 11	5	11	131.618	0.31373	261.888	1000.	0.	0.009703	-0.824979
S 11	5	12	171.011	0.191088	128.635	1505.13	0.0000314829	0.0100059	-2.51198
S 11	5	13	148.938	0.162949	253.127	1000.	3.1129731680475602' 10 ⁻⁶	0.00704428	-0.273772
S 11	5	14	103.464	0.0377938	649.322	911.152	-0.0000206584	0.00863202	-2.84815
S 11	5	15	52.087	0.331342	250.185	900.282	-3.1362218793415093' 10 ⁻⁶	0.00400681	1.53895
S 11	5	16	81.4743	0.180716	585.322	1129.75	0.0000166388	0.00588171	1.81033
S 11	5	17	76.2247	0.0878382	362.485	1604.55	-0.0000149294	0.00508533	-0.218643
S 11	5	18	36.0082	0.301808	602.435	995.069	-7.42294' 10 ⁻⁷	0.00227077	0.620605
S 11	5	19	100.457	0.274362	216.935	999.926	7.81743' 10 ⁻⁶	0.00471674	-2.12505
S 11	5	20	24.69	0.22227	493.467	878.801	-1.6897662722253736' 10 ⁻⁶	0.00139539	-2.61889

Sample 11 Scan 6:

S	T	M	LL	w	s	t	a	% erg	f
S 11	6	1	825.553	0.0262859	225.854	1027.63	0.0000631776	0.562007	0.0856923
S 11	6	2	183.58	0.00701766	520.767	1596.19	-1.98572 ' 10 ⁻⁶	0.0733131	-0.509702
S 11	6	3	170.922	0.084257	240.024	968.064	-0.0000163341	0.0446004	-1.01229
S 11	6	4	322.149	0.103223	232.167	934.96	-0.0000249099	0.0607171	-0.496633
S 11	6	5	140.21	0.165523	429.623	1099.81	-0.0000288168	0.0337865	0.399541
S 11	6	6	99.2508	0.0663244	457.342	754.892	-0.0000136346	0.021209	2.63953
S 11	6	7	517.975	0.190595	44.3408	900.108	-6.27637 ' 10 ⁻⁷	0.060079	0.903113
S 11	6	8	69.9869	0.0260015	134.018	1139.4	0.000115118	0.00967832	-0.82671
S 11	6	9	137.886	0.237275	84.8364	1199.64	1.1987040767150602 ' 10 ⁻⁶	0.0166055	1.76094
S 11	6	10	166.148	0.313957	266.52	1000.01	-7.40331 ' 10 ⁻⁷	0.0117708	-0.765072
S 11	6	11	207.647	0.13563	229.45	899.974	5.07426 ' 10 ⁻⁶	0.0104561	-0.0857003
S 11	6	12	109.769	0.274543	263.649	999.969	0.	0.00789862	-2.08979
S 11	6	13	101.197	0.0364366	634.414	899.808	-0.0000245616	0.00835089	-2.06275
S 11	6	14	92.5783	0.192657	741.493	1345.72	-0.0000279622	0.00693297	-2.16118
S 11	6	15	50.7804	0.0445518	723.67	1228.92	0.0000250747	0.00353889	-1.49556
S 11	6	16	47.3887	0.331321	278.576	961.903	2.50828 ' 10 ⁻⁶	0.00314291	-0.144306
S 11	6	17	76.7568	0.102691	289.134	1643.02	0.0000287967	0.00478694	3.02624
S 11	6	18	80.3958	0.162118	241.772	1119.99	-0.0000138111	0.00462547	-0.16029
S 11	6	19	45.382	0.303144	866.88	1071.51	-8.4884 ' 10 ⁻⁶	0.00245693	-2.83629
S 11	6	20	67.0102	0.22928	317.769	857.437	-8.43238 ' 10 ⁻⁶	0.00342995	1.12619

Sample 11 Scan 7:

S	T	M	LL	w	s	t	a	% erg	f
S 11	7	1	823.48	0.0262973	225.944	1027.11	0.0000633181	0.561098	0.0852068
S 11	7	2	181.387	0.00700816	518.653	1595.36	-1.93627 ' 10 ⁻⁶	0.0726678	-0.512008
S 11	7	3	251.933	0.0884815	78.0538	845.536	0.0000774016	0.081316	2.31116
S 11	7	4	157.194	0.166253	250.79	1000.	6.31873 ' 10 ⁻⁷	0.0291543	-2.72906
S 11	7	5	230.147	0.190663	36.1583	904.28	0.000385876	0.052354	-0.223922
S 11	7	6	140.052	0.0991884	251.392	1000.	-2.80688 ' 10 ⁻⁷	0.0216343	-2.06214
S 11	7	7	100.941	0.0519975	439.006	766.728	0.0000228482	0.017347	3.02726
S 11	7	8	107.661	0.112625	244.026	1000.	5.72335 ' 10 ⁻⁸	0.0133585	-1.022
S 11	7	9	104.785	0.236857	253.877	1102.07	-4.61369 ' 10 ⁻⁶	0.0149038	-0.0753922
S 11	7	10	47.9144	0.0883501	822.006	1411.36	-1.2926573350193622 ' 10 ⁻⁶	0.00631889	-2.40101
S 11	7	11	166.907	0.314225	207.055	1000.	-1.1996502471492275 ' 10 ⁻⁶	0.0133735	-0.77728
S 11	7	12	139.912	0.162968	-56.1731	1000.	2.62075 ' 10 ⁻⁷	0.0122675	-0.503116
S 11	7	13	85.628	0.0229584	540.637	966.721	8.0923 ' 10 ⁻⁶	0.00846109	3.09291
S 11	7	14	130.172	0.183997	125.573	1499.37	0.	0.0104079	-1.23292
S 11	7	15	79.8163	0.055712	131.303	1390.45	0.0000947061	0.00646193	-1.36103
S 11	7	16	118.568	0.27409	202.318	1000.	5.07464 ' 10 ⁻⁶	0.00686591	-2.15464
S 11	7	17	67.439	0.204028	102.379	1199.63	-4.00582 ' 10 ⁻⁶	0.00459788	1.6465
S 11	7	18	82.8563	0.329555	212.111	947.778	-0.0000530114	0.00372488	-0.863389
S 11	7	19	63.7844	0.106304	199.123	1580.43	-5.224 ' 10 ⁻⁷	0.00386716	-2.60481
S 11	7	20	34.5581	0.163037	1093.51	1757.11	-4.97339 ' 10 ⁻⁷	0.00199444	2.8474

Sample 11 Scan 8:

S	T	M	LL	w	s	t	a	% erg	f
S 11	8	1	808.073	0.0263327	225.83	1026.63	0.000063338	0.554284	0.0905156
S 11	8	2	173.223	0.00700697	515.28	1592.96	-1.9515736297086244 ' 10 ⁻⁶	0.0707582	-0.493563
S 11	8	3	250.678	0.0889009	77.2228	845.355	0.0000777647	0.0828937	2.31226
S 11	8	4	518.095	0.190713	46.6654	900.003	-6.81865 ' 10 ⁻⁷	0.083432	0.859653
S 11	8	5	205.001	0.0978573	106.657	1100.01	3.1396545203695316 ' 10 ⁻⁶	0.0313338	0.399781
S 11	8	6	103.415	0.0520335	440.404	765.514	0.0000226229	0.0173108	3.0938
S 11	8	7	151.715	0.237119	225.515	1100.	3.1457446022357064 ' 10 ⁻⁶	0.0140907	0.370361
S 11	8	8	151.994	0.314594	167.317	1100.	-2.3700124261865146 ' 10 ⁻⁸	0.012874	-0.671856
S 11	8	9	81.8273	0.196971	110.749	1500.01	1.1978661077624558 ' 10 ⁻⁶	0.0103055	-1.49483
S 11	8	10	71.0587	0.0230384	538.412	962.112	8.07872 ' 10 ⁻⁶	0.00834189	-3.08223
S 11	8	11	179.403	0.169951	203.582	1100.	-0.0000145675	0.0115488	0.127087
S 11	8	12	76.5613	0.0557695	22.905	1397.48	-0.0000862239	0.00749744	-1.64857
S 11	8	13	101.18	0.274246	262.225	969.818	5.09053 ' 10 ⁻⁶	0.00900511	-0.0988759
S 11	8	14	143.104	0.140531	171.372	900.	0.0000356941	0.00963557	-0.189205
S 11	8	15	72.2589	0.211583	179.845	1213.42	-9.98502 ' 10 ⁻⁷	0.00489788	-1.29194
S 11	8	16	55.7576	0.301818	508.901	984.379	-7.59767 ' 10 ⁻⁶	0.00383339	-1.46652
S 11	8	17	40.5558	0.221839	1377.95	1586.93	2.41559 ' 10 ⁻⁶	0.002657	1.62018
S 11	8	18	62.9543	0.0888568	951.011	1947.96	0.0000170989	0.00391678	-0.498719
S 11	8	19	38.1246	0.0814927	1409.34	1227.68	-1.3950953486762136 ' 10 ⁻⁶	0.00225481	-0.969864
S 11	8	20	23.5172	0.0202726	359.875	1644.17	7.17534 ' 10 ⁻⁶	0.00134861	-2.97859

Sample 11 Scan 9:

S	T	M	LL	w	s	t	a	% erg	f
S 11	9	1	809.099	0.026343	225.461	1026.4	0.000063399	0.554741	0.0908738
S 11	9	2	173.383	0.00699692	516.876	1592.5	-1.92825 ' 10 ⁻⁶	0.0707473	-0.494475
S 11	9	3	255.413	0.0888551	77.6111	845.329	0.000078506	0.0841719	2.31361
S 11	9	4	373.645	0.190708	42.917	900.133	-1.1590876028305054 ' 10 ⁻⁶	0.0843473	0.841932
S 11	9	5	205.353	0.0977672	109.159	1100.	2.6920102957270044 ' 10 ⁻⁷	0.0302037	0.410591
S 11	9	6	105.77	0.0521985	439.042	762.285	0.0000227331	0.017535	-3.03009
S 11	9	7	110.704	0.237457	238.792	1100.	2.4955618066215718 ' 10 ⁻⁸	0.0156536	0.405265
S 11	9	8	145.015	0.31483	172.382	1100.	1.17489 ' 10 ⁻⁶	0.01198	-0.690169
S 11	9	9	66.9233	0.0230827	535.186	960.357	8.08797 ' 10 ⁻⁶	0.00838532	-3.04576
S 11	9	10	93.5785	0.196707	119.448	1500.	-3.6963225664015914 ' 10 ⁻⁶	0.0107512	-1.48903
S 11	9	11	160.48	0.170005	208.397	1100.	-0.0000166615	0.011874	0.156099
S 11	9	12	79.2287	0.0557404	24.7225	1397.41	-0.0000414884	0.00750488	-1.65742
S 11	9	13	90.1899	0.273625	261.274	1000.	0.	0.00760233	-1.90301
S 11	9	14	200.511	0.127397	70.6195	984.061	0.0000298893	0.0111834	0.806156
S 11	9	15	85.7776	0.212141	219.2	1100.	-4.49774 ' 10 ⁻⁸	0.00423131	-2.26093
S 11	9	16	89.1332	0.101958	85.0007	1674.71	-0.000141678	0.00579897	0.123037
S 11	9	17	66.7847	0.301972	420.161	1006.69	-5.80364 ' 10 ⁻⁶	0.00401854	-2.03152
S 11	9	18	25.0179	0.0202384	372.598	1643.87	7.1191041913165775 ' 10 ⁻⁶	0.0014376	-2.99059
S 11	9	19	34.3943	0.221173	2469.44	2294.72	1.0906186913153365 ' 10 ⁻⁶	0.00191858	2.
S 11	9	20	53.6173	0.0485937	1478.75	1089.05	9.65912 ' 10 ⁻⁷	0.00286232	2.4487

Sample 11 Scan 10:

S	T	M	LL	w	s	t	a	% erg	f
S 11	10	1	803.287	0.0263537	225.366	1026.39	0.0000633828	0.552146	0.0926143
S 11	10	2	171.25	0.00700129	516.9	1591.09	-1.9404314456317194 ' 10 ⁻⁶	0.0703579	-0.484385
S 11	10	3	251.095	0.0888304	78.1907	845.186	0.0000843875	0.0835854	2.32029
S 11	10	4	363.176	0.190873	40.5386	902.057	0.000266063	0.0891794	0.356012
S 11	10	5	90.1729	0.0523995	434.335	759.319	0.0000231113	0.0175609	-2.90118
S 11	10	6	133.609	0.0986875	160.925	1000.	5.99718 ' 10 ⁻⁸	0.0200079	-2.10523
S 11	10	7	125.037	0.237989	302.279	1086.54	-0.0000132262	0.0195215	-2.44388
S 11	10	8	64.4637	0.0874983	727.092	1282.77	-4.96418 ' 10 ⁻⁷	0.00915025	2.34115
S 11	10	9	86.4822	0.113248	264.686	1000.	0.	0.0112434	-0.820101
S 11	10	10	96.3192	0.196354	117.572	1499.49	-4.08076 ' 10 ⁻⁶	0.0112497	-1.39176
S 11	10	11	178.353	0.314423	239.653	1100.	1.50471 ' 10 ⁻⁷	0.0110839	-0.585127
S 11	10	12	205.209	0.169767	192.506	1099.79	-0.0000205898	0.0123165	0.324582
S 11	10	13	95.7363	0.0231445	527.991	956.851	8.22602 ' 10 ⁻⁶	0.00835586	-2.9727
S 11	10	14	82.8889	0.0555773	125.124	1392.29	0.0000999687	0.00661578	-1.48678
S 11	10	15	49.964	0.302332	507.196	1021.15	-7.14043 ' 10 ⁻⁶	0.00373086	-0.271912
S 11	10	16	97.3147	0.223932	54.1799	1200.39	1.8538524183630554 ' 10 ⁻⁶	0.00618573	1.26306
S 11	10	17	93.7313	0.274188	271.955	1020.36	0.0000331567	0.00594993	-1.74599
S 11	10	18	56.9325	0.329847	406.211	1041.79	6.5236 ' 10 ⁻⁶	0.00335846	-1.53035
S 11	10	19	80.5574	0.105112	152.795	1612.82	-9.30371 ' 10 ⁻⁶	0.00443699	0.319244
S 11	10	20	46.2312	0.0480535	532.316	743.288	-5.41362 ' 10 ⁻⁶	0.0023895	1.09799

Sample 11 Scan 11:

S	T	M	LL	w	s	t	a	% erg	f
S 11	11	1	802.198	0.0263711	224.977	1026.38	0.0000632419	0.551658	0.100409
S 11	11	2	170.061	0.00698845	519.068	1590.6	-1.97274 ' 10 ⁻⁶	0.0699883	-0.47067
S 11	11	3	251.303	0.0889479	76.8322	844.999	0.0000847513	0.0838406	2.34554
S 11	11	4	562.463	0.190994	44.1628	899.995	-1.9596436673988834 ' 10 ⁻⁶	0.090041	0.880817
S 11	11	5	124.005	0.0979394	189.453	1000.	-1.0885248195933514 ' 10 ⁻⁷	0.0180123	-2.1856
S 11	11	6	101.438	0.0522667	437.645	760.976	0.000022811	0.0178846	-2.95762
S 11	11	7	136.07	0.236461	70.4082	1199.76	1.1509889484576553 ' 10 ⁻⁶	0.020671	1.74849
S 11	11	8	54.169	0.0876019	816.121	1322.77	-8.36766 ' 10 ⁻⁷	0.00774302	-1.03002
S 11	11	9	137.676	0.113382	146.415	1000.	-1.2187215398819232 ' 10 ⁻⁹	0.0141635	-0.80976
S 11	11	10	69.9432	0.0230335	535.808	961.533	8.05494 ' 10 ⁻⁶	0.00844021	-3.06147
S 11	11	11	172.471	0.176447	440.959	1290.64	-0.0000290145	0.0184558	-0.803185
S 11	11	12	74.7557	0.0562022	147.523	1390.48	0.000107936	0.00706219	-1.4177
S 11	11	13	276.525	0.312036	118.901	1000.	5.44772 ' 10 ⁻⁷	0.0129804	-0.485641
S 11	11	14	116.543	0.27461	244.285	1000.	-1.9382053890030102 ' 10 ⁻⁶	0.00725517	-2.09724
S 11	11	15	120.054	0.19163	675.5	1322.35	-0.0000277421	0.00800316	2.4161
S 11	11	16	92.4012	0.229834	345.214	867.984	-8.12384 ' 10 ⁻⁶	0.00553763	-1.33778
S 11	11	17	91.1589	0.106154	235.602	1565.28	0.0000145666	0.00498404	-1.10796
S 11	11	18	130.562	0.138967	209.642	900.	-1.93821 ' 10 ⁻⁶	0.00520705	0.0982366
S 11	11	19	53.6367	0.0482597	553.02	759.564	-5.74513 ' 10 ⁻⁶	0.00245519	0.343459
S 11	11	20	51.5221	0.33032	242.74	900.	-0.0000322741	0.00216155	2.53164

Sample 11 Scan 12:

S	T	M	LL	W	S	t	a	% erg	f
S 11	12	1	823.318	0.0264219	224.695	1026.45	0.0000631206	0.561027	0.111109
S 11	12	2	176.532	0.0069991	516.521	1589.98	-2.0045565469870263 ' 10 ⁻⁶	0.0709036	-0.459181
S 11	12	3	270.343	0.0892416	76.0961	844.813	0.0000797498	0.0869307	2.40726
S 11	12	4	539.585	0.190889	51.4627	900.306	8.09912 ' 10 ⁻⁶	0.0884631	0.926077
S 11	12	5	126.585	0.0978796	222.503	999.996	-1.1978812205940977 ' 10 ⁻⁶	0.0179088	-2.17625
S 11	12	6	93.3028	0.0598815	186.596	587.428	2.69643 ' 10 ⁻⁶	0.0154714	0.820078
S 11	12	7	47.3151	0.0877495	848.409	1334.05	-5.63527 ' 10 ⁻⁷	0.00731112	-1.99409
S 11	12	8	100.709	0.112544	517.438	1162.98	5.87646 ' 10 ⁻⁶	0.0144561	-0.516978
S 11	12	9	67.2329	0.0286074	98.2495	1140.72	0.0000410021	0.00887146	-0.681402
S 11	12	10	155.948	0.236163	56.9163	1199.75	-1.8631907318882845 ' 10 ⁻⁶	0.0176156	1.78593
S 11	12	11	143.87	0.191968	132.55	1506.76	-0.0000382132	0.0143181	-2.46312
S 11	12	12	111.416	0.168349	160.368	1100.	-3.82921 ' 10 ⁻⁷	0.00828986	0.232159
S 11	12	13	105.423	0.274973	224.729	1000.31	1.2039005687226186 ' 10 ⁻⁶	0.00727072	-2.03683
S 11	12	14	150.441	0.143002	109.989	999.996	8.64672 ' 10 ⁻⁸	0.00961824	-1.1557
S 11	12	15	128.737	0.0306057	250.24	725.09	-0.0000305699	0.00850906	-2.7448
S 11	12	16	308.785	0.312404	-96.2621	1000.	-1.9396335055704004 ' 10 ⁻⁶	0.0112165	-0.364616
S 11	12	17	156.891	0.060756	149.924	1387.72	0.000209864	0.00736361	-1.55962
S 11	12	18	102.129	0.230762	401.908	921.956	-7.31117 ' 10 ⁻⁶	0.00420737	-1.22689
S 11	12	19	56.6559	0.104686	337.937	733.431	-3.30546 ' 10 ⁻⁶	0.00215524	2.39886
S 11	12	20	55.1913	0.206259	192.526	719.857	-0.000025058	0.00197202	-3.10439

Sample 11 Scan 13:

S	T	M	LL	W	S	t	a	% erg	f
S 11	13	1	1162.9	0.022124	239.312	1060.86	0.0000632794	0.687421	-0.55145
S 11	13	2	329.763	0.00698984	554.215	1596.68	-2.5657161553944113 ' 10 ⁻⁶	0.0875983	-0.411815
S 11	13	3	352.103	0.0848904	81.9485	853.266	0.000123813	0.0665152	1.97258
S 11	13	4	100.791	0.0594063	193.84	589.426	-3.1760389600945336 ' 10 ⁻⁶	0.0151103	1.04847
S 11	13	5	393.03	0.19097	45.8547	900.	-6.99349 ' 10 ⁻⁷	0.0419278	1.24149
S 11	13	6	127.783	0.0985586	208.893	1000.08	-7.3372 ' 10 ⁻⁷	0.0118338	-1.71054
S 11	13	7	64.0219	0.0877513	833.486	1340.39	-6.29527 ' 10 ⁻⁷	0.00550242	-2.1773
S 11	13	8	108.888	0.0229714	548.116	902.099	8.04642 ' 10 ⁻⁶	0.00858616	-1.26035
S 11	13	9	117.871	0.0476548	526.679	1162.39	-0.0000193018	0.00829892	-1.0907
S 11	13	10	130.409	0.112539	555.255	1157.22	5.98665 ' 10 ⁻⁶	0.00811087	0.486045
S 11	13	11	156.75	0.237245	239.754	1099.99	-6.1579 ' 10 ⁻⁶	0.00615248	0.903064
S 11	13	12	126.992	0.194843	147.04	1510.49	-0.0000453781	0.0062103	-2.90244
S 11	13	13	111.714	0.0266233	250.109	1508.45	0.0000174701	0.00484798	0.504283
S 11	13	14	166.261	0.169115	139.307	1100.	-1.4925316108882747 ' 10 ⁻⁷	0.0036739	0.548957
S 11	13	15	58.5304	0.216629	270.364	1063.82	-0.000014909	0.00212235	0.0340753
S 11	13	16	143.776	0.143215	249.94	1000.01	-1.93821 ' 10 ⁻⁶	0.00368458	-1.01273
S 11	13	17	45.139	0.0399671	3767.65	7708.35	3.202 ' 10 ⁻⁷	0.00139188	-2.32563
S 11	13	18	203.914	0.31567	238.203	1100.	-2.1822039622323164 ' 10 ⁻⁶	0.0030812	-0.457645
S 11	13	19	68.2227	0.102096	854.254	1224.01	3.99093 ' 10 ⁻⁶	0.00178476	1.79273
S 11	13	20	151.268	0.272585	216.973	1000.31	0.0000279733	0.00301999	-2.00251

Sample 11 Scan 14:

S	T	M	LL	W	S	t	a	% erg	f
S 11	14	1	1312.95	0.0212491	240.077	1070.59	0.0000626107	0.730976	-0.670826
S 11	14	2	448.54	0.00700479	555.969	1597.02	-2.68948427779907805 ' 10 ⁻⁶	0.0969416	-0.383696
S 11	14	3	316.743	0.0844915	83.777	850.624	0.000123024	0.0464614	2.34226
S 11	14	4	112.995	0.0596191	191.496	589.523	-6.3709329126843495 ' 10 ⁻⁶	0.0133212	1.23575
S 11	14	5	392.105	0.191047	49.0295	900.	5.8428 ' 10 ⁻⁷	0.0323142	1.2204
S 11	14	6	146.968	0.0275595	783.051	728.686	-0.0000250233	0.0108035	-2.6544
S 11	14	7	124.561	0.0981218	197.692	1000.05	-4.98786 ' 10 ⁻⁶	0.00796522	-1.61735
S 11	14	8	109.933	0.0181898	569.401	1403.72	-6.2092165129321855 ' 10 ⁻⁶	0.00626652	2.57537
S 11	14	9	70.9778	0.0875321	792.539	1291.07	-6.82384 ' 10 ⁻⁷	0.00369491	2.25626
S 11	14	10	93.874	0.0307388	469.845	1278.21	-0.0000145907	0.00450088	1.89477
S 11	14	11	123.63	0.113301	221.426	1000.	1.2391384704017949 ' 10 ⁻⁶	0.00397244	-0.418899
S 11	14	12	180.91	0.236571	-60.3612	1200.	8.35349 ' 10 ⁻⁷	0.00602987	1.99702
S 11	14	13	148.726	0.192727	143.353	1499.28	-0.000037825	0.00493629	-0.746211
S 11	14	14	88.1751	0.0472878	951.282	1247.46	-0.0000125744	0.00259883	0.444624
S 11	14	15	144.685	0.168586	141.958	1099.92	-1.9327441960126343 ' 10 ⁻⁶	0.00259718	0.540287
S 11	14	16	236.202	0.316413	160.405	1099.79	-1.93821 ' 10 ⁻⁶	0.00286918	-0.354725
S 11	14	17	136.813	0.143376	197.383	999.989	2.9638470333872844 ' 10 ⁻⁶	0.00231914	-1.04243
S 11	14	18	89.0797	0.274612	280.729	1000.31	1.1979301616470875 ' 10 ⁻⁶	0.0017318	-1.87477
S 11	14	19	125.067	0.230097	151.765	1000.	-2.75944 ' 10 ⁻⁶	0.00144387	-0.0908747
S 11	14	20	125.069	0.104581	186.775	1595.09	9.90639 ' 10 ⁻⁶	0.00202586	2.59325

Sample 11 Scan 15:

S	T	M	LL	w	s	t	a	% erg	f
S 11 15	1	1226.29	0.0219245	238.92	1064.02	0.0000629101		0.706621	-0.576577
S 11 15	2	371.785	0.00699984	552.367	1595.52	-2.67937' 10 ⁻⁶		0.0908473	-0.384939
S 11 15	3	344.892	0.083856	84.4609	854.313	0.000125876		0.0588075	1.9734
S 11 15	4	111.281	0.0594395	192.064	590.018	-4.50452' 10 ⁻⁶		0.0150379	1.10098
S 11 15	5	409.745	0.190438	47.3386	900.108	3.1364156295713237' 10 ⁻⁶		0.0394072	1.26448
S 11 15	6	126.909	0.0985843	194.842	1000.	-0.0000134225		0.010458	-1.4876
S 11 15	7	78.2475	0.0876376	813.984	1287.34	-7.12284' 10 ⁻⁷		0.00586234	2.59785
S 11 15	8	130.061	0.0229207	543.072	904.576	8.05046' 10 ⁻⁶		0.00878436	-1.26599
S 11 15	9	134.548	0.047315	541.632	1154.39	-0.0000193384		0.0079616	-0.644591
S 11 15	10	166.353	0.236665	-67.1298	1200.	-7.40338' 10 ⁻⁷		0.00710454	2.02843
S 11 15	11	123.939	0.113655	119.728	1000.	3.13609' 10 ⁻⁶		0.00460005	-0.408328
S 11 15	12	126.461	0.025413	270.95	1529.96	0.0000151571		0.00517657	0.0492046
S 11 15	13	237.519	0.192782	131.606	1481.28	0.0000131952		0.00498366	2.52154
S 11 15	14	46.0668	0.0365248	3846.2	8100.08	5.44093' 10 ⁻⁷		0.00150447	-0.354842
S 11 15	15	161.505	0.169428	137.36	1100.	9.16247' 10 ⁻⁷		0.00301491	0.591062
S 11 15	16	104.108	0.144347	236.882	1000.04	-1.3351105146595675' 10 ⁻⁷		0.00251719	-1.19392
S 11 15	17	107.016	0.104565	202.497	1588.31	0.0000104034		0.00267723	-2.98545
S 11 15	18	409.557	0.316392	97.9309	1000.	8.20315' 10 ⁻⁶		0.00427285	-0.0961969
S 11 15	19	95.7084	0.274343	281.63	988.942	2.3110946355088825' 10 ⁻⁶		0.00177241	1.2388
S 11 15	20	177.777	0.22989	182.365	1000.	-4.4631' 10 ⁻⁶		0.00169709	0.0169607

Sample 11 Scan 16:

S	T	M	LL	w	s	t	a	% erg	f
S 11 16	1	999.711	0.022866	237.633	1053.04	0.0000638671		0.632014	-0.448616
S 11 16	2	238.48	0.00700904	547.181	1593.96	-2.59442' 10 ⁻⁶		0.0779409	-0.411945
S 11 16	3	355.72	0.0865312	78.2303	852.953	0.000126595		0.0865874	1.85199
S 11 16	4	415.508	0.190012	-48.734	900.	-2.82906' 10 ⁻⁷		0.0642272	1.29733
S 11 16	5	130.021	0.0592498	192.22	588.744	-1.23849' 10 ⁻⁶		0.0168808	0.938962
S 11 16	6	143.03	0.0987995	209.807	1000.	-1.9676726385292436' 10 ⁻⁷		0.0155133	-1.79627
S 11 16	7	70.64	0.0877714	888.335	1371.2	-6.43145' 10 ⁻⁷		0.00723364	1.3342
S 11 16	8	152.785	0.113925	199.48	1000.	1.65543' 10 ⁻⁶		0.0106148	-0.465797
S 11 16	9	102.796	0.0226329	578.628	921.947	7.3880484804703234' 10 ⁻⁶		0.0086174	-1.72012
S 11 16	10	116.896	0.0478457	525.138	1165.47	-0.0000192706		0.00878108	-1.38831
S 11 16	11	197.716	0.23639	-56.1966	1200.	1.1978812205938682' 10 ⁻⁶		0.0108423	2.00792
S 11 16	12	301.91	0.185921	137.543	1464.1	-0.0000466571		0.00819237	-0.242756
S 11 16	13	121.29	0.165668	223.941	1100.34	0.		0.0036404	0.445057
S 11 16	14	210.229	0.143935	177.077	900.	-2.0662236647838533' 10 ⁻⁶		0.00631654	0.558443
S 11 16	15	104.936	0.104831	192.681	1596.56	9.80051' 10 ⁻⁶		0.00416622	2.28297
S 11 16	16	115.239	0.0261574	289.594	1515.39	0.0000144814		0.00409872	0.321813
S 11 16	17	53.6204	0.0418403	3440.43	6979.23	-0.0000102693		0.00175194	0.57919
S 11 16	18	320.041	0.317483	165.076	1100.	4.3344' 10 ⁻⁶		0.00478604	-0.271608
S 11 16	19	47.2298	0.0425003	1125.98	1717.83	1.5223704550477675' 10 ⁻⁶		0.00124639	-2.79825
S 11 16	20	116.141	0.275031	258.89	1010.56	-7.83243' 10 ⁻⁷		0.0025767	1.64661

Sample 11 Scan 17:

S	T	M	LL	w	s	t	a	% erg	f
S 11 17	1	835.034	0.0264598	224.132	1026.98	0.0000630025		0.56614	0.115192
S 11 17	2	179.364	0.00699797	516.551	1589.51	-2.0868' 10 ⁻⁶		0.0710959	-0.447477
S 11 17	3	440.664	0.0849899	99.1411	800.	-2.0990844057361525' 10 ⁻⁶		0.0667945	0.188013
S 11 17	4	442.041	0.190395	60.1339	899.975	3.1710065437412177' 10 ⁻⁶		0.0924839	1.18776
S 11 17	5	185.853	0.108135	345.673	983.833	-3.74958' 10 ⁻⁶		0.0343189	0.554806
S 11 17	6	189.037	0.0757281	623.406	876.381	-0.0000233979		0.0289418	-0.249363
S 11 17	7	58.1355	0.0481081	451.088	1070.65	1.1124927992124435' 10 ⁻⁶		0.00785526	2.16856
S 11 17	8	120.186	0.197521	305.863	1366.39	0.00002784		0.0148611	-0.644162
S 11 17	9	105.644	0.0288129	413.892	1193.33	-0.000234775		0.0116666	-1.01179
S 11 17	10	176.883	0.170163	222.462	1099.2	-0.0000323995		0.010149	0.610756
S 11 17	11	66.7957	0.0887352	338.797	1613.79	-0.0000136023		0.0061028	-0.710263
S 11 17	12	196.514	0.23632	116.009	1200.	3.13646' 10 ⁻⁶		0.0123927	2.1194
S 11 17	13	99.3976	0.0280274	245.387	691.88	-0.0000148431		0.00718667	-2.00167
S 11 17	14	271.251	0.141928	135.358	899.933	-5.22834' 10 ⁻⁷		0.0119234	0.430536
S 11 17	15	35.3678	0.175555	216.509	800.	-0.0000277703		0.00196867	-1.06433
S 11 17	16	266.782	0.317002	148.61	1100.	-7.38418' 10 ⁻⁷		0.00707682	-0.180733
S 11 17	17	94.2727	0.272692	247.788	1000.51	3.5211235251907676' 10 ⁻⁶		0.00422955	-1.70051
S 11 17	18	123.12	0.0610061	1032.31	1226.41	7.5986230459395756' 10 ⁻⁶		0.00504724	1.97858
S 11 17	19	60.414	0.301768	400.437	982.983	-2.92979' 10 ⁻⁶		0.00225841	-1.08699
S 11 17	20	64.6194	0.0175989	306.034	1561.8	-0.0000178598		0.00226927	-0.823936

Sample 11 Scan 18:

S	T	M	LL	w	s	t	a	% erg	f
S 11	18	1	737.05	0.0234598	236.115	1043.99	0.0000648521	0.521477	-0.376162
S 11	18	2	139.085	0.00695802	551.468	1588.17	-2.3041984415333526 ' 10 ⁻⁶	0.0620711	-0.432746
S 11	18	3	514.404	0.190451	50.3432	900.	-1.5758474662590137 ' 10 ⁻⁸	0.122732	0.903983
S 11	18	4	382.673	0.0868742	75.7408	848.136	0.000100518	0.0932104	1.95316
S 11	18	5	80.8743	0.0593859	195.719	586.987	7.29878 ' 10 ⁻⁶	0.0155332	0.751266
S 11	18	6	133.894	0.099814	215.373	1000.	-1.94053 ' 10 ⁻⁶	0.0190699	-2.10245
S 11	18	7	51.3629	0.0879505	851.494	1368.14	-6.04629 ' 10 ⁻⁷	0.00827764	1.34468
S 11	18	8	138.105	0.236395	234.044	1100.	5.41314 ' 10 ⁻⁷	0.0146342	0.484025
S 11	18	9	151.005	0.198885	321.09	1344.11	0.0000331802	0.0199614	-2.84267
S 11	18	10	102.099	0.111659	587.043	1235.9	6.36385 ' 10 ⁻⁶	0.0118861	-2.55586
S 11	18	11	174.533	0.144795	145.48	900.003	-7.59393 ' 10 ⁻⁶	0.0142793	0.0799888
S 11	18	12	82.933	0.022703	557.851	920.152	7.70848 ' 10 ⁻⁶	0.00766387	-1.84277
S 11	18	13	100.978	0.0478289	517.376	1161.11	-0.0000190682	0.00851276	-1.41318
S 11	18	14	108.254	0.305129	265.418	938.94	-0.0000186935	0.00821664	-0.643956
S 11	18	15	40.8446	0.209164	397.24	846.073	-0.0000189975	0.00287764	2.38674
S 11	18	16	118.226	0.170736	379.315	1097.39	-0.000014565	0.00769655	0.710908
S 11	18	17	110.459	0.272247	240.07	1000.	3.13234 ' 10 ⁻⁶	0.00583684	-1.89068
S 11	18	18	75.3242	0.327938	213.429	900.	3.13609 ' 10 ⁻⁶	0.00390519	1.39373
S 11	18	19	47.3818	0.103574	417.416	742.838	-3.3250444852678647 ' 10 ⁻⁶	0.00238722	1.62421
S 11	18	20	78.2589	0.171041	923.763	1890.	0.0000458124	0.00370342	0.486603

Sample 11 Scan 19:

S	T	M	LL	w	s	t	a	% erg	f
S 11	19	1	727.311	0.0264698	224.572	1024.19	0.0000635056	0.516794	0.10813
S 11	19	2	141.685	0.00697084	522.48	1583.84	-2.14937 ' 10 ⁻⁶	0.0637342	-0.423824
S 11	19	3	453.871	0.190752	57.1753	900.	2.9293546022344665 ' 10 ⁻⁶	0.12084	0.876936
S 11	19	4	343.527	0.084197	114.707	865.479	0.0000102814	0.0725138	0.662676
S 11	19	5	287.964	0.107039	174.798	1100.	3.5448249234734407 ' 10 ⁻⁸	0.0355775	0.212254
S 11	19	6	84.1834	0.0607951	154.986	568.001	-6.0229613858947164 ' 10 ⁻⁶	0.0152796	1.91846
S 11	19	7	110.044	0.193823	241.691	1457.26	0.0000112098	0.018163	0.485845
S 11	19	8	139.809	0.236574	83.1887	1200.	3.9912 ' 10 ⁻⁸	0.0202698	1.64244
S 11	19	9	56.9555	0.0254959	621.775	916.595	-2.11903 ' 10 ⁻⁶	0.00752217	-1.51761
S 11	19	10	76.9911	0.100126	433.285	1363.81	-0.0000156976	0.00951063	1.15419
S 11	19	11	221.713	0.143357	133.515	900.001	-8.21821 ' 10 ⁻⁶	0.0204986	0.16677
S 11	19	12	128.934	0.170187	166.546	1099.92	-4.2499733637956934 ' 10 ⁻⁶	0.00805318	0.116903
S 11	19	13	47.7806	0.0164198	728.456	1281.74	-2.95603 ' 10 ⁻⁶	0.00421234	-2.67406
S 11	19	14	129.408	0.0464999	445.575	1134.62	-0.0000179543	0.0104477	-0.291479
S 11	19	15	161.949	0.109271	201.01	799.831	-1.1918589695221292 ' 10 ⁻⁶	0.00639059	0.486753
S 11	19	16	110.49	0.30507	246.964	900.	-0.0000209229	0.0072074	-1.22944
S 11	19	17	121.055	0.0828033	443.049	1521.61	-0.0000288835	0.00707173	0.946793
S 11	19	18	90.4192	0.272988	333.074	989.782	3.2952071384520146 ' 10 ⁻⁶	0.0047508	0.791169
S 11	19	19	131.744	0.228429	174.328	999.926	-4.97388 ' 10 ⁻⁶	0.003226	-0.261055
S 11	19	20	84.2759	0.327489	204.184	900.097	1.3013716645763958 ' 10 ⁻⁶	0.00365806	1.37474

Sample 11 Scan 20:

S	T	M	LL	w	s	t	a	% erg	f
S 11	20	1	714.89	0.0264872	224.26	1024.28	0.000063392	0.510754	0.112911
S 11	20	2	139.617	0.00697183	521.57	1584.05	-2.1087769073912414 ' 10 ⁻⁶	0.0636547	-0.426592
S 11	20	3	424.574	0.190055	59.0421	899.998	-1.05746 ' 10 ⁻⁹	0.11944	0.927283
S 11	20	4	363.669	0.0911036	72.917	841.81	0.0000977525	0.093046	2.51003
S 11	20	5	93.5614	0.0980877	221.686	1000.	3.17664 ' 10 ⁻⁶	0.0156737	-2.37921
S 11	20	6	83.8694	0.059838	186.466	582.982	3.6633550656149212 ' 10 ⁻⁶	0.0158058	0.993764
S 11	20	7	41.1559	0.0876661	964.945	1397.07	-6.6818 ' 10 ⁻⁷	0.0072845	-1.28231
S 11	20	8	121.945	0.194279	272.931	1442.56	0.0000112827	0.0199046	-2.80931
S 11	20	9	104.129	0.112233	557.44	1194.49	6.27368 ' 10 ⁻⁶	0.0151773	2.14852
S 11	20	10	185.671	0.236141	75.0746	1199.69	5.26571 ' 10 ⁻⁷	0.0226175	1.76212
S 11	20	11	252.181	0.145529	151.191	900.	2.0719540810980123 ' 10 ⁻⁸	0.0186814	0.255244
S 11	20	12	86.3551	0.0290102	99.7892	1136.55	0.0000451008	0.00802491	-0.604703
S 11	20	13	156.774	0.178014	136.794	1100.	1.5304281985428763 ' 10 ⁻⁷	0.00886159	0.400534
S 11	20	14	110.038	0.0304948	244.503	724.716	-0.000027887	0.00834691	-2.83494
S 11	20	15	95.1409	0.304922	250.079	900.107	-0.0000169639	0.00649472	-1.31997
S 11	20	16	72.1891	0.273148	320.028	998.815	1.8269148263258746 ' 10 ⁻⁶	0.00454506	-1.56501
S 11	20	17	136.428	0.0584097	126.082	1391.4	0.000130526	0.00774319	-1.56058
S 11	20	18	56.0201	0.207069	255.528	765.837	-1.34087 ' 10 ⁻⁶	0.00288562	-0.249399
S 11	20	19	62.8664	0.229362	363.632	860.542	-4.9686 ' 10 ⁻⁶	0.0030515	0.18154
S 11	20	20	92.1168	0.327557	215.261	900.615	6.56472 ' 10 ⁻⁶	0.0037659	1.24966

Sample 11 Scan 21:

S	T	M	LL	w	s	t	a	% erg	f
S 11	21	1	723.156	0.0235331	235.576	1043.6	0.0000645272	0.514781	-0.356733
S 11	21	2	136.649	0.00695427	549.354	1582.98	-2.46538' 10 ⁻⁶	0.0619123	-0.378041
S 11	21	3	148.803	0.189421	235.545	900.	-1.0803899646330207' 10 ⁻⁷	0.0558146	0.965684
S 11	21	4	309.223	0.0904401	70.8221	845.022	0.000130049	0.0975956	2.18054
S 11	21	5	248.968	0.166688	57.2468	900.	-1.9087' 10 ⁻⁶	0.0508732	0.821159
S 11	21	6	74.5235	0.193185	503.186	989.006	-0.000012368	0.0156883	-0.420209
S 11	21	7	80.978	0.0596829	186.914	580.743	2.1998' 10 ⁻⁶	0.0157725	1.14727
S 11	21	8	124.678	0.0987433	201.009	1000.	0.	0.0159854	-2.23565
S 11	21	9	52.3192	0.0875308	883.143	1310.87	-3.8706518495779906' 10 ⁻⁷	0.00871706	-0.0463887
S 11	21	10	94.0778	0.189064	185.19	1508.4	-0.0000221516	0.0145719	-2.79106
S 11	21	11	152.905	0.211582	203.613	800.096	4.00776' 10 ⁻⁶	0.0114632	-2.71519
S 11	21	12	154.623	0.114483	220.653	1000.12	-7.50082' 10 ⁻¹⁰	0.013699	-0.830136
S 11	21	13	233.11	0.233393	74.875	1199.67	1.1744222105791696' 10 ⁻⁶	0.0241513	1.80901
S 11	21	14	63.9702	0.167006	351.239	923.235	-4.06896' 10 ⁻⁶	0.00609799	-1.83362
S 11	21	15	84.9819	0.0226641	559.367	921.573	7.72452' 10 ⁻⁶	0.00752051	-1.88211
S 11	21	16	111.611	0.0476513	508.75	1158.39	-0.0000190032	0.00895432	-1.27913
S 11	21	17	211.986	0.305251	98.2398	1000.	-3.26704' 10 ⁻⁷	0.00821781	-0.481859
S 11	21	18	95.5517	0.105243	201.408	1598.96	0.0000124409	0.00616178	1.66397
S 11	21	19	137.517	0.145785	166.733	900.	5.07462' 10 ⁻⁶	0.00526804	-0.221498
S 11	21	20	72.0064	0.272542	334.724	948.247	7.73174' 10 ⁻⁶	0.00390356	-0.471381

Sample 11 Scan 22:

S	T	M	LL	w	s	t	a	% erg	f
S 11	22	1	705.752	0.0265198	223.554	1024.3	0.0000630681	0.506263	0.12874
S 11	22	2	138.22	0.0069746	521.974	1581.4	-2.09736' 10 ⁻⁶	0.0636436	-0.39712
S 11	22	3	464.569	0.189217	48.606	900.	-4.44794' 10 ⁻⁷	0.12778	0.998207
S 11	22	4	380.894	0.0905089	75.8541	841.616	0.0000870454	0.0954655	2.56443
S 11	22	5	120.043	0.0981628	208.188	1000.02	-1.9382165747768534' 10 ⁻⁶	0.0165601	-2.26665
S 11	22	6	88.2245	0.0600217	177.348	576.398	1.6182115434345117' 10 ⁻⁶	0.0159908	1.39354
S 11	22	7	49.2336	0.0875363	906.473	1339.29	-4.7414' 10 ⁻⁷	0.00832912	-2.53128
S 11	22	8	201.915	0.236527	45.0344	1199.77	2.7054129833592705' 10 ⁻⁶	0.0295089	1.72178
S 11	22	9	115.918	0.112295	597.497	1182.47	6.4259' 10 ⁻⁶	0.0148346	-2.82091
S 11	22	10	128.807	0.191905	161.872	1504.89	6.3227' 10 ⁻⁶	0.0145875	-2.2584
S 11	22	11	71.6243	0.0255193	646.744	929.564	-2.11825' 10 ⁻⁶	0.00733454	-1.83006
S 11	22	12	183.141	0.145305	159.174	900.	8.20327' 10 ⁻⁶	0.0118516	-0.0286868
S 11	22	13	49.996	0.0163366	707.745	1267.	-3.09755' 10 ⁻⁶	0.00423918	-2.41808
S 11	22	14	98.2631	0.0394824	250.666	947.735	-0.0000119088	0.00768293	1.20153
S 11	22	15	133.671	0.23144	251.521	1000.	-1.8693634433225678' 10 ⁻⁶	0.00544073	-0.548325
S 11	22	16	75.2733	0.167773	387.473	999.588	-0.000013653	0.00504414	-1.62984
S 11	22	17	73.0515	0.275475	128.73	1100.	4.38285' 10 ⁻⁶	0.00434242	1.78987
S 11	22	18	97.2654	0.304585	230.043	899.93	-0.0000104401	0.00522427	-1.3077
S 11	22	19	120.275	0.0608668	114.039	1377.39	0.0000743783	0.00622758	-0.532229
S 11	22	20	67.3545	0.10201	970.75	1205.28	3.9315' 10 ⁻⁶	0.00317385	-3.08012

Sample 11 Scan 23:

S	T	M	LL	w	s	t	a	% erg	f
S 11	23	1	708.55	0.0265481	223.057	1023.83	0.0000631046	0.507642	0.132202
S 11	23	2	139.256	0.00695688	522.986	1580.33	-2.0109921389523017' 10 ⁻⁶	0.0639103	-0.401891
S 11	23	3	283.266	0.18772	126.207	870.854	-3.58034' 10 ⁻⁶	0.0753409	0.161033
S 11	23	4	332.606	0.0922846	69.2238	839.323	0.0000652831	0.0996514	2.78426
S 11	23	5	75.8413	0.0975708	206.03	999.926	-8.78212' 10 ⁻¹⁰	0.0153387	-2.42595
S 11	23	6	169.892	0.164737	267.877	1000.05	-9.50752' 10 ⁻⁶	0.0252992	-2.67209
S 11	23	7	78.4387	0.0597781	160.268	564.748	-3.04693' 10 ⁻⁶	0.0159852	2.12262
S 11	23	8	100.736	0.211837	227.003	866.274	4.11073' 10 ⁻⁶	0.018246	2.31259
S 11	23	9	110.924	0.193758	292.43	1443.35	0.0000122675	0.0186541	-2.93197
S 11	23	10	52.7162	0.0874686	909.656	1337.73	-4.2199389533461346' 10 ⁻⁷	0.00816561	-2.41903
S 11	23	11	106.773	0.111745	588.841	1232.08	6.52769' 10 ⁻⁶	0.0152767	-2.04583
S 11	23	12	215.992	0.233144	78.6675	1200.	1.4347319027257846' 10 ⁻⁷	0.0242121	1.87512
S 11	23	13	256.545	0.145174	168.126	900.	-1.9382118553057415' 10 ⁻⁶	0.0192284	0.389066
S 11	23	14	84.542	0.0255113	637.935	920.997	-1.98182' 10 ⁻⁶	0.00746898	-1.64639
S 11	23	15	202.844	0.176835	189.898	737.049	-7.76377' 10 ⁻⁷	0.00797199	-3.00851
S 11	23	16	154.383	0.0455432	457.8	1110.	-0.0000174396	0.0109713	0.778862
S 11	23	17	67.2706	0.0163369	718.902	1268.89	-3.1312022205436967' 10 ⁻⁶	0.00427566	-2.45336
S 11	23	18	175.916	0.304768	101.6	1000.	2.83627' 10 ⁻⁶	0.00598929	-0.403741
S 11	23	19	68.6612	0.101825	883.075	1214.15	4.4486328325134135' 10 ⁻⁶	0.00367989	2.09735
S 11	23	20	44.3783	0.128195	281.45	941.597	7.64099' 10 ⁻⁶	0.00224742	0.219774

Sample 11 Scan 24:

S	T	M	LL	w	s	t	a	% erg	f
S 11	24	1	698.076	0.0265475	223.495	1023.45	0.0000631244	0.502458	0.131445
S 11	24	2	136.299	0.00695015	523.84	1578.84	-2.0381542763241603 ' 10 ⁻⁶	0.0633034	-0.39114
S 11	24	3	434.141	0.190007	63.3593	900.	3.13512 ' 10 ⁻⁶	0.119358	0.977703
S 11	24	4	386.892	0.0920834	71.0234	839.973	0.0000868718	0.100732	2.67203
S 11	24	5	94.9023	0.0979942	233.411	1000.	3.1353149931930074 ' 10 ⁻⁶	0.0147031	-2.45705
S 11	24	6	86.0936	0.0600021	172.087	572.77	1.78908 ' 10 ⁻⁶	0.0163771	1.59625
S 11	24	7	91.8548	0.111936	560.819	1210.9	6.6287324327986806 ' 10 ⁻⁶	0.0159863	0.266406
S 11	24	8	129.893	0.194245	282.968	1438.48	0.0000168405	0.0202411	-2.07049
S 11	24	9	41.7838	0.0868282	331.422	1614.68	-0.0000173676	0.00597177	-0.9254
S 11	24	10	216.187	0.235395	96.0347	1200.	1.1978812205938682 ' 10 ⁻⁶	0.0252787	1.85082
S 11	24	11	66.3931	0.0255355	643.741	922.967	-2.0497863828243496 ' 10 ⁻⁶	0.00736651	-1.69521
S 11	24	12	234.747	0.14554	138.174	900.108	-1.8902188479974533 ' 10 ⁻⁶	0.0191302	0.251345
S 11	24	13	189.997	0.170334	180.753	1100.	-0.0000240694	0.00878325	0.236698
S 11	24	14	54.3294	0.0163043	739.175	1269.71	-2.9337664868177027 ' 10 ⁻⁶	0.00419849	-2.48928
S 11	24	15	153.8	0.0453161	463.736	1107.41	-0.0000168251	0.01072	0.835429
S 11	24	16	45.242	0.104285	664.784	929.736	1.7923015628449305 ' 10 ⁻⁶	0.00285212	0.315022
S 11	24	17	70.9366	0.0876626	424.628	922.84	-5.99631 ' 10 ⁻⁶	0.0042201	2.69966
S 11	24	18	61.2429	0.206556	220.5	739.172	0.0000117929	0.0034102	-1.15301
S 11	24	19	164.093	0.303671	109.452	1000.	4.9663 ' 10 ⁻⁶	0.00529525	-0.51401
S 11	24	20	52.7237	0.132413	405.111	1734.25	-0.000127996	0.00250116	-0.246163

Sample 11 Scan 25:

S	T	M	LL	w	s	t	a	% erg	f
S 11	25	1	695.007	0.0265476	223.82	1023.41	0.000063149	0.500929	0.133105
S 11	25	2	134.466	0.00693573	524.573	1576.46	-2.11167 ' 10 ⁻⁶	0.0627017	-0.36692
S 11	25	3	486.931	0.189706	46.2674	900.	4.6184788952219183 ' 10 ⁻⁷	0.129535	0.964204
S 11	25	4	390.882	0.0909029	75.4475	840.959	0.0000849072	0.0989816	2.58855
S 11	25	5	114.037	0.0982273	215.093	1000.	-1.9387995864844876 ' 10 ⁻⁶	0.0164637	-2.30331
S 11	25	6	90.372	0.0600559	170.8	571.947	1.1703451784687805 ' 10 ⁻⁶	0.0164596	1.65169
S 11	25	7	49.775	0.0876211	941.071	1362.32	-6.10688 ' 10 ⁻⁷	0.00845019	1.73667
S 11	25	8	123.932	0.194467	287.77	1444.4	0.00001827	0.0192997	3.10484
S 11	25	9	197.791	0.236243	97.3157	1200.	2.8533 ' 10 ⁻⁶	0.0240807	1.87571
S 11	25	10	135.475	0.112151	608.545	1188.46	6.64076 ' 10 ⁻⁶	0.0154822	2.7325
S 11	25	11	72.2855	0.0255719	649.015	927.894	-2.0969362707214144 ' 10 ⁻⁶	0.00744173	-1.81591
S 11	25	12	176.808	0.143984	153.546	900.	-1.7766940116818315 ' 10 ⁻⁶	0.0118831	-0.0629814
S 11	25	13	48.1592	0.0162767	729.464	1260.91	-3.0142651873731025 ' 10 ⁻⁶	0.00410889	-2.34134
S 11	25	14	134.83	0.0456262	463.842	1117.52	-0.0000175498	0.0105047	0.415922
S 11	25	15	115.073	0.169874	-97.8564	1100.	-1.93842 ' 10 ⁻⁶	0.00535054	0.433896
S 11	25	16	83.8238	0.228233	243.031	900.	6.0784 ' 10 ⁻⁶	0.00538603	-2.51512
S 11	25	17	50.9534	0.207635	308.522	786.765	9.8043 ' 10 ⁻⁶	0.00308194	1.63266
S 11	25	18	59.0707	0.101977	935.552	1207.21	4.18097 ' 10 ⁻⁶	0.0033818	2.8899
S 11	25	19	102.135	0.302795	179.565	900.542	-1.7286311467901172 ' 10 ⁻⁶	0.00523375	-1.74783
S 11	25	20	60.798	0.329421	243.45	900.175	0.0000127356	0.00293518	1.24231

Sample 11 Scan 26:

S	T	M	LL	w	s	t	a	% erg	f
S 11	26	1	697.815	0.0265579	223.935	1023.32	0.0000633817	0.502329	0.129637
S 11	26	2	135.185	0.0069492	524.535	1577.86	-2.0654947151701003 ' 10 ⁻⁶	0.0628389	-0.385243
S 11	26	3	284.865	0.188162	253.939	1007.27	-9.38602 ' 10 ⁻⁵	0.0561982	-0.189666
S 11	26	4	318.776	0.0925517	69.708	839.254	0.0000715555	0.103111	2.75656
S 11	26	5	275.887	0.167082	175.974	1000.	-1.9706084752615495 ' 10 ⁻⁶	0.0411435	-2.83636
S 11	26	6	233.094	0.205026	197.712	1000.	-1.1993333311115945 ' 10 ⁻⁶	0.0305224	-0.694294
S 11	26	7	122.592	0.0977491	254.905	1000.	2.17002 ' 10 ⁻⁸	0.0146079	-2.46325
S 11	26	8	91.274	0.0599727	163.983	564.928	1.2131117713587844 ' 10 ⁻⁶	0.0164312	2.07948
S 11	26	9	48.247	0.0877809	978.016	1406.23	-8.69683 ' 10 ⁻⁷	0.00809829	-2.00152
S 11	26	10	106.36	0.111139	588.694	1251.87	6.79847 ' 10 ⁻⁶	0.0165307	1.95177
S 11	26	11	215.008	0.145494	198.398	899.933	5.05039 ' 10 ⁻⁹	0.0193408	0.394973
S 11	26	12	195.671	0.232235	118.119	1200.	5.07201 ' 10 ⁻⁶	0.0199936	1.95152
S 11	26	13	136.464	0.188327	164.897	1506.46	-0.0000139816	0.0137727	-2.40713
S 11	26	14	84.4102	0.0255653	649.75	923.551	-2.00514 ' 10 ⁻⁶	0.00762475	-1.72997
S 11	26	15	80.4511	0.175019	331.071	870.589	-0.0000138021	0.00669191	-0.660531
S 11	26	16	54.1945	0.0162498	731.258	1254.61	-3.13158 ' 10 ⁻⁶	0.00421378	-2.21307
S 11	26	17	158.858	0.0469275	463.205	1148.19	-0.0000180086	0.0111139	-0.968204
S 11	26	18	74.443	0.216473	503.48	950.051	5.0820685508906234 ' 10 ⁻⁶	0.00463087	2.44872
S 11	26	19	49.6229	0.129426	295.328	926.132	0.000011693	0.00290085	2.21688
S 11	26	20	49.3748	0.159156	344.394	1031.9	-2.4089808191081052 ' 10 ⁻⁶	0.00274695	0.368922

Sample 11 Scan 27:

S	T	M	LL	w	s	t	a	% erg	f
S 11	27	1	708.826	0.0265504	224.229	1023.27	0.0000637223	0.507778	0.118562
S 11	27	2	138.594	0.0069538	521.874	1577.42	-2.0305907309365547' 10 ⁻⁶	0.06361	-0.395641
S 11	27	3	281.664	0.092787	69.5406	838.659	0.0000704157	0.10499	2.80851
S 11	27	4	679.498	0.182776	46.6244	917.225	-0.0000309866	0.12645	-2.10419
S 11	27	5	120.489	0.0979746	201.306	1000.	6.85866' 10 ⁻⁸	0.0149318	-2.41038
S 11	27	6	98.8354	0.0598325	162.248	563.959	2.7123542868067893' 10 ⁻⁷	0.0170648	2.14392
S 11	27	7	56.782	0.0874985	935.991	1338.54	-5.16077' 10 ⁻⁷	0.00906769	-2.4849
S 11	27	8	113.53	0.11176	647.43	1212.23	6.75349' 10 ⁻⁶	0.0166567	0.0743585
S 11	27	9	153.167	0.194875	401.439	1411.29	0.0000131799	0.0196753	-2.88921
S 11	27	10	67.9071	0.0256188	647.329	923.101	-1.9148097279193726' 10 ⁻⁶	0.00780412	-1.73663
S 11	27	11	126.952	0.169438	412.198	1025.5	-0.0000126513	0.0132417	0.31891
S 11	27	12	178.607	0.224175	66.0293	1200.	3.4188751470306183' 10 ⁻⁶	0.0149634	1.83759
S 11	27	13	54.2528	0.0162871	737.881	1259.84	-3.1293437886512886' 10 ⁻⁶	0.00437562	-2.30776
S 11	27	14	158.504	0.0468659	460.798	1147.36	-0.0000177545	0.0115043	-0.944431
S 11	27	15	57.7117	0.101734	882.048	1228.78	4.6201021383778774' 10 ⁻⁶	0.00375612	0.572394
S 11	27	16	67.0172	0.208019	283.944	1218.59	2.25915' 10 ⁻⁶	0.00409824	1.12961
S 11	27	17	99.2587	0.302561	175.542	900.19	-0.0000238779	0.00548766	-1.43528
S 11	27	18	90.5433	0.243698	209.557	1100.	1.9382125294060955' 10 ⁻⁶	0.0041081	1.20155
S 11	27	19	48.4323	0.197881	331.765	765.532	0.0000433357	0.00234169	0.470482
S 11	27	20	55.1424	0.329978	259.152	900.108	4.0836' 10 ⁻⁶	0.00253025	1.40025

Sample 11 Scan 28:

S	T	M	LL	w	s	t	a	% erg	f
S 11	28	1	693.066	0.026613	223.368	1023.08	0.0000635131	0.499959	0.131726
S 11	28	2	135.002	0.00697147	519.754	1578.58	-1.99604' 10 ⁻⁶	0.0630581	-0.405254
S 11	28	3	430.79	0.186643	55.999	908.631	-0.0000239783	0.12731	-0.505597
S 11	28	4	411.473	0.091889	73.4724	840.074	0.0000793544	0.104156	2.6926
S 11	28	5	126.582	0.0981119	204.065	999.999	5.94061' 10 ⁻⁹	0.016349	-2.35796
S 11	28	6	94.4714	0.0600384	163.897	568.079	-5.5470182837932873' 10 ⁻⁸	0.0169712	1.90337
S 11	28	7	55.5214	0.0881068	190.37	1634.86	-0.000175974	0.00925118	-2.08204
S 11	28	8	125.913	0.194207	311.409	1435.15	0.0000138432	0.0191708	-1.1895
S 11	28	9	60.0984	0.0254521	694.194	976.594	-1.94846' 10 ⁻⁶	0.00833333	-2.99269
S 11	28	10	45.4411	0.0876972	742.855	1105.78	-5.32423' 10 ⁻⁷	0.00597666	-1.09587
S 11	28	11	113.189	0.112633	487.263	1132.19	6.94943' 10 ⁻⁶	0.0137582	2.84364
S 11	28	12	239.938	0.237418	96.0202	1199.97	-1.57956' 10 ⁻⁶	0.0210374	1.98817
S 11	28	13	124.679	0.048985	509.015	1169.79	-0.0000225611	0.010991	-1.8872
S 11	28	14	158.357	0.170297	176.834	1100.	-6.27633' 10 ⁻⁶	0.00900877	0.136975
S 11	28	15	46.9284	0.0165948	825.442	1317.	-2.00976' 10 ⁻⁶	0.00338167	2.81191
S 11	28	16	115.114	0.143905	258.796	1000.	-4.82969' 10 ⁻⁸	0.00729006	-1.74371
S 11	28	17	121.489	0.326923	255.579	989.41	0.0000388897	0.00377777	2.94896
S 11	28	18	116.855	0.302639	258.158	1000.	0.	0.00354546	-0.389147
S 11	28	19	65.4377	0.272966	282.949	979.572	7.68932' 10 ⁻⁶	0.00353191	-2.9591
S 11	28	20	135.491	0.519833	260.519	1000.	2.0703331718727345' 10 ⁻⁶	0.00500111	-0.965637

Sample 11 Scan 29:

S	T	M	LL	w	s	t	a	% erg	f
S 11	29	1	695.38	0.0235143	235.343	1043.13	0.0000651608	0.501115	-0.374502
S 11	29	2	129.742	0.00697267	543.309	1581.54	-2.3914166208617766' 10 ⁻⁶	0.0606482	-0.395312
S 11	29	3	286.324	0.0917758	70.068	843.42	0.000116956	0.108977	2.33344
S 11	29	4	766.218	0.182946	47.3495	918.373	-0.000023274	0.128352	-2.22867
S 11	29	5	114.56	0.0992662	202.654	1000.	3.1358618929066816' 10 ⁻⁶	0.0163914	-2.27502
S 11	29	6	97.0919	0.0595034	168.829	572.265	1.3578242903836436' 10 ⁻⁶	0.0170224	1.66994
S 11	29	7	55.4974	0.0875297	903.245	1338.07	-4.5002694794232977' 10 ⁻⁷	0.00901291	-2.41601
S 11	29	8	112.622	0.196699	763.391	1298.56	8.89309' 10 ⁻⁶	0.0168222	0.640312
S 11	29	9	127.314	0.111431	672.494	1243.74	7.00493' 10 ⁻⁶	0.0168694	2.86718
S 11	29	10	164.937	0.223396	49.1378	1199.91	-1.8969552795985112' 10 ⁻⁶	0.0168278	1.93822
S 11	29	11	73.9385	0.0229833	552.782	903.892	7.75766' 10 ⁻⁶	0.00765579	-1.47671
S 11	29	12	46.2958	0.190932	665.509	1209.29	6.42044' 10 ⁻⁶	0.00451329	-2.76113
S 11	29	13	118.997	0.168639	409.614	989.64	-0.0000120044	0.0106859	0.055128
S 11	29	14	116.082	0.0476463	505.531	1159.48	-0.0000187036	0.0092679	-1.3329
S 11	29	15	74.1606	0.21748	203.607	800.001	3.16381' 10 ⁻⁶	0.00283749	3.07291
S 11	29	16	60.6818	0.327529	273.268	990.581	0.0000401598	0.00425571	2.56126
S 11	29	17	104.118	0.30317	239.757	1000.	-7.41783' 10 ⁻⁷	0.00381444	-0.409518
S 11	29	18	69.7209	0.273407	277.765	1000.	2.7729267250989928' 10 ⁻⁶	0.00433363	-2.19111
S 11	29	19	60.209	0.118037	688.718	1219.15	0.0000370565	0.00350907	2.45147
S 11	29	20	44.6618	0.206797	563.845	1238.73	-6.0963997791752265' 10 ⁻⁶	0.00246981	3.11169

Sample 11 Scan 30:

S	T	M	LL	w	s	t	a	% erg	f
S 11	30	1	696.625	0.0265987	222.907	1023.3	0.0000638111	0.501736	0.117883
S 11	30	2	137.279	0.00698941	514.754	1581.22	-1.9107248662711327' 10 ⁻⁶	0.0638218	-0.438162
S 11	30	3	288.656	0.093112	69.487	838.663	0.000062469	0.108694	2.8507
S 11	30	4	776.223	0.183699	49.4111	910.094	-0.00004049	0.119895	-0.672604
S 11	30	5	109.491	0.0976072	250.047	1000.	-2.02232' 10 ⁻⁹	0.014314	-2.46874
S 11	30	6	96.8916	0.0594996	153.416	557.023	-4.44655' 10 ⁻⁶	0.0175978	2.60376
S 11	30	7	66.3146	0.0997721	80.9683	1676.85	-0.0000427507	0.0110906	-0.0768607
S 11	30	8	122.14	0.113453	197.77	1000.	1.0413055593822616' 10 ⁻⁶	0.0145783	-0.976555
S 11	30	9	138.479	0.194331	355.197	1420.38	0.0000125192	0.0190539	1.79862
S 11	30	10	66.0564	0.0256778	676.371	935.525	-2.0289952657166607' 10 ⁻⁶	0.00820034	-2.01844
S 11	30	11	52.575	0.0878882	576.198	1027.85	-1.7533872271608754' 10 ⁻⁶	0.00615043	-0.355017
S 11	30	12	109.433	0.170629	431.261	1070.37	-0.0000115341	0.0118103	-1.05236
S 11	30	13	112.803	0.0446935	448.46	1094.07	-0.0000147503	0.0108941	1.40602
S 11	30	14	46.5551	0.0163971	750.636	1280.12	-2.9217703253202843' 10 ⁻⁶	0.00414993	-2.70131
S 11	30	15	237.553	0.238696	85.3387	1200.01	3.1360938060868168' 10 ⁻⁶	0.0159058	1.97917
S 11	30	16	76.6266	0.321451	284.544	1037.73	0.0000398749	0.00524956	-0.166248
S 11	30	17	87.4114	0.300103	211.174	867.394	-0.0000119111	0.00413787	2.1974
S 11	30	18	139.197	0.143865	147.464	900.	0.	0.00661847	-0.213204
S 11	30	19	86.6977	0.273125	319.996	988.146	2.7134587812993103' 10 ⁻⁶	0.00458158	1.16865
S 11	30	20	51.5223	0.113886	157.12	1400.12	4.03099' 10 ⁻⁷	0.00248747	-1.73944

Sample 11 Scan 31:

S	T	M	LL	w	s	t	a	% erg	f
S 11	31	1	701.431	0.0266004	222.96	1023.28	0.0000638736	0.504125	0.11609
S 11	31	2	139.285	0.00697319	516.798	1580.75	-1.8480176212523275' 10 ⁻⁶	0.0643796	-0.442332
S 11	31	3	296.071	0.0933832	69.0739	838.745	0.0000626298	0.110338	2.85146
S 11	31	4	368.781	0.185531	251.933	993.413	-0.0000358673	0.054876	3.12005
S 11	31	5	155.034	0.20286	271.933	1038.35	-7.5527662696554335' 10 ⁻⁶	0.0380685	-1.75878
S 11	31	6	82.8203	0.0977744	205.907	1000.	3.1359' 10 ⁻⁶	0.0145094	-2.46701
S 11	31	7	172.763	0.0593019	139.345	544.617	-2.23485' 10 ⁻⁶	0.0177565	-2.93925
S 11	31	8	60.0216	0.0993989	91.7391	1682.48	-7.23177' 10 ⁻⁶	0.0113605	-0.672096
S 11	31	9	159.212	0.167202	251.522	1073.43	-0.0000248298	0.0266265	-1.82404
S 11	31	10	89.8277	0.190842	205.138	1500.1	5.27336' 10 ⁻⁷	0.0134902	-0.862143
S 11	31	11	148.378	0.11364	139.196	1000.	5.0745606928608165' 10 ⁻⁶	0.0138906	-0.818671
S 11	31	12	66.8264	0.0257122	678.93	936.604	-1.97078' 10 ⁻⁶	0.00838052	-2.056
S 11	31	13	56.1722	0.0883001	512.374	1043.27	-1.7263796215747705' 10 ⁻⁶	0.00662384	-1.83182
S 11	31	14	146.723	0.144952	170.477	999.878	-2.74034' 10 ⁻⁶	0.0155022	-1.4746
S 11	31	15	112.531	0.0449544	451.964	1100.37	-0.0000155602	0.0105512	1.15052
S 11	31	16	98.9522	0.216554	479.285	838.983	-0.000028657	0.00834604	2.55252
S 11	31	17	53.2231	0.0163719	758.63	1278.85	-2.90717' 10 ⁻⁶	0.00415896	-2.69461
S 11	31	18	90.7685	0.329517	198.922	953.663	0.0000437715	0.00526535	2.09881
S 11	31	19	78.7783	0.2722	235.175	1000.	3.74105' 10 ⁻⁶	0.00475713	-1.93624
S 11	31	20	99.4693	0.185652	229.466	910.76	0.00001365	0.00376696	-0.597481

Sample 11 Scan 32:

S	T	M	LL	w	s	t	a	% erg	f
S 11	32	1	709.91	0.0265673	223.041	1023.34	0.0000638389	0.508312	0.110306
S 11	32	2	142.876	0.00698029	518.12	1579.03	-1.8968635941420676' 10 ⁻⁶	0.0653641	-0.430067
S 11	32	3	304.693	0.0932954	69.4654	838.585	0.0000640405	0.111728	2.85019
S 11	32	4	478.781	0.177869	221.123	870.446	-0.0000366871	0.0629115	0.261606
S 11	32	5	86.7504	0.0977079	231.656	1000.	-1.9432505282643046' 10 ⁻⁶	0.0144294	-2.44032
S 11	32	6	80.695	0.0600991	154.793	562.281	-4.6838952442113826' 10 ⁻⁷	0.0183164	2.26378
S 11	32	7	190.092	0.205043	249.915	1000.	-4.12572' 10 ⁻⁸	0.0224311	-0.598605
S 11	32	8	69.324	0.192838	594.404	1187.42	-4.00918' 10 ⁻⁶	0.0130985	-2.98003
S 11	32	9	300.867	0.157449	122.928	1000.	-7.34408' 10 ⁻⁷	0.0340647	-2.25141
S 11	32	10	80.4107	0.0996354	87.7034	1680.57	-0.0000215422	0.0114606	-0.464631
S 11	32	11	64.3503	0.025722	681.387	940.18	-1.9197369458332857' 10 ⁻⁶	0.00853502	-2.15742
S 11	32	12	132.085	0.113759	145.747	1000.02	1.1861726698429825' 10 ⁻⁶	0.0125559	-0.798885
S 11	32	13	63.3474	0.0880685	514.322	1019.02	-2.1557058312015193' 10 ⁻⁶	0.00711152	0.385528
S 11	32	14	57.0947	0.16372	432.986	925.592	-4.21939' 10 ⁻⁶	0.00603479	2.03061
S 11	32	15	42.3217	0.0163284	751.436	1270.51	-2.9089029357989236' 10 ⁻⁶	0.00425613	-2.55341
S 11	32	16	116.276	0.0445329	459.136	1087.08	-0.0000148203	0.0108073	1.69686
S 11	32	17	180.713	0.232938	99.4654	1200.	-4.4865' 10 ⁻⁶	0.0118866	2.05784
S 11	32	18	163.298	0.140023	221.974	1000.	-1.98585' 10 ⁻⁶	0.00827938	-0.688312
S 11	32	19	111.738	0.184263	652.476	1589.84	-8.4879' 10 ⁻⁶	0.00713406	1.04537
S 11	32	20	88.379	0.329533	236.62	945.172	0.0000437566	0.00502909	-1.44809

Sample 11 Scan 33:

S	T	M	LL	w	s	t	a	% erg	f
S 11	33	1	721.483	0.0265426	222.717	1023.59	0.0000639627	0.513969	0.10236
S 11	33	2	147.818	0.00696992	519.414	1575.27	-1.9323395724103926 ' 10 ⁻⁶	0.0666855	-0.408236
S 11	33	3	521.67	0.136819	99.41	871.588	-0.000480622	0.170075	-0.566824
S 11	33	4	87.8148	0.0869891	676.619	1094.47	-1.2240763183469783 ' 10 ⁻⁶	0.0208774	0.181069
S 11	33	5	86.6276	0.192381	444.906	1202.68	-8.60227 ' 10 ⁻⁶	0.0188747	0.682459
S 11	33	6	204.18	0.110198	184.955	1100.34	-1.7179843308240873 ' 10 ⁻⁸	0.0267185	0.30593
S 11	33	7	138.819	0.0518072	407.492	723.933	0.0000128119	0.0235722	-0.0981888
S 11	33	8	184.946	0.133069	166.429	900.	1.2464212829979956 ' 10 ⁻⁷	0.0220196	-1.08572
S 11	33	9	151.235	0.172194	647.932	1137.99	-0.0000131463	0.0191264	0.0388625
S 11	33	10	81.5517	0.0306529	511.869	1130.3	-0.0000991591	0.00917426	0.0193774
S 11	33	11	44.555	0.0153068	934.814	969.814	-4.5215823435929824 ' 10 ⁻⁷	0.00470503	1.44973
S 11	33	12	100.778	0.0720455	241.973	906.734	-0.0000125314	0.00986817	-2.4378
S 11	33	13	106.392	0.226184	376.83	1103.42	-0.0000126431	0.00942633	-1.21377
S 11	33	14	191.668	0.246899	220.198	1098.22	-4.85002 ' 10 ⁻⁶	0.0117245	2.09436
S 11	33	15	127.73	0.110986	74.9146	1686.28	-0.000132596	0.0086629	-0.70377
S 11	33	16	64.2494	0.042913	1075.82	1451.39	1.6806512125798446 ' 10 ⁻⁷	0.00395668	2.18949
S 11	33	17	106.967	0.329557	223.349	942.623	0.0000430132	0.00404651	-0.561545
S 11	33	18	70.0793	0.174435	437.12	865.808	-0.000011769	0.00376158	1.14862
S 11	33	19	63.2442	0.0647956	163.346	1387.31	-2.25806 ' 10 ⁻⁶	0.00316737	-0.402838
S 11	33	20	45.95	0.107232	286.733	683.555	0.0000223833	0.00218488	-0.250053

Sample 11 Scan 34:

S	T	M	LL	w	s	t	a	% erg	f
S 11	34	1	722.062	0.0265391	223.287	1023.17	0.000064137	0.514251	0.0966749
S 11	34	2	148.218	0.00696207	520.668	1574.68	-1.8897225537085075 ' 10 ⁻⁶	0.0668121	-0.414413
S 11	34	3	525.345	0.136894	98.9912	871.337	-0.000480291	0.170816	-0.577022
S 11	34	4	87.3816	0.0869565	678.058	1089.28	-1.18931 ' 10 ⁻⁶	0.020682	0.591129
S 11	34	5	197.781	0.110071	189.287	1100.	1.55037 ' 10 ⁻⁶	0.0276807	0.326265
S 11	34	6	97.1974	0.189125	455.531	1103.75	-0.0000198536	0.0184149	1.20521
S 11	34	7	139.565	0.0518777	409.959	722.352	0.0000130101	0.0234997	-0.0418248
S 11	34	8	174.311	0.132833	153.022	899.996	3.15851 ' 10 ⁻⁸	0.0211282	-1.11606
S 11	34	9	102.609	0.16849	286.398	987.32	-0.0000101563	0.0132373	0.325982
S 11	34	10	76.1533	0.0257525	535.087	1105.88	-0.0000987439	0.00898499	0.686417
S 11	34	11	43.6994	0.0153074	828.327	1018.25	-5.01328 ' 10 ⁻⁷	0.00485521	0.720768
S 11	34	12	92.1772	0.0716626	248.782	915.914	-0.0000108635	0.00955988	3.13426
S 11	34	13	101.955	0.225852	396.277	1091.05	-0.0000122022	0.00960906	1.49522
S 11	34	14	133.695	0.24757	249.042	1099.28	-4.86233 ' 10 ⁻⁶	0.0111722	1.72109
S 11	34	15	96.9169	0.187741	212.929	1537.44	-4.83035 ' 10 ⁻⁶	0.00723731	-1.79297
S 11	34	16	128.405	0.11153	75.9693	1687.3	-0.000143813	0.00856958	-0.813471
S 11	34	17	65.8705	0.0428534	1084.4	1463.32	1.8291874529894744 ' 10 ⁻⁷	0.00398715	1.6699
S 11	34	18	138.365	0.315463	174.703	1100.	1.1436478291201147 ' 10 ⁻⁶	0.00537763	-0.873427
S 11	34	19	61.2697	0.0651591	166.424	1391.34	-2.5231306364643216 ' 10 ⁻⁶	0.00315764	-0.713725
S 11	34	20	43.091	0.107307	278.25	688.066	0.000023017	0.00210973	-0.750001

Sample 11 Scan 35:

S	T	M	LL	w	s	t	a	% erg	f
S 11	35	1	714.119	0.0265879	223.038	1022.99	0.0000640576	0.510377	0.105743
S 11	35	2	146.769	0.0069986	514.469	1578.37	-1.8434701318674945 ' 10 ⁻⁶	0.0667342	-0.443933
S 11	35	3	389.059	0.0871052	152.565	808.338	-0.000394492	0.135991	0.0259997
S 11	35	4	249.848	0.148489	140.07	961.768	0.000283787	0.0630297	-3.08669
S 11	35	5	95.2651	0.0868781	600.243	1111.94	6.05881 ' 10 ⁻⁷	0.0201787	-1.91264
S 11	35	6	161.318	0.0542112	331.718	800.988	-0.0000158918	0.0300769	-2.66821
S 11	35	7	101.234	0.196086	410.551	1386.07	0.0000160126	0.0165417	2.1342
S 11	35	8	73.3635	0.0136908	887.104	916.38	-5.24435 ' 10 ⁻⁶	0.0109833	-2.81163
S 11	35	9	102.599	0.108525	607.127	1110.97	-4.45252 ' 10 ⁻⁶	0.0140634	-0.678242
S 11	35	10	99.8527	0.0679404	402.937	707.496	-0.0000120661	0.012369	-1.27415
S 11	35	11	104.741	0.230985	57.7407	1200.	1.1975243775424786 ' 10 ⁻⁶	0.0110398	1.82061
S 11	35	12	79.9342	0.0997022	263.088	1659.36	8.91698 ' 10 ⁻⁷	0.00820094	1.81628
S 11	35	13	103.178	0.168036	475.498	989.973	-0.000015005	0.00966125	0.35997
S 11	35	14	74.3126	0.0556212	149.505	1400.	3.13609 ' 10 ⁻⁶	0.0059953	-1.41517
S 11	35	15	50.3798	0.0257313	157.195	1222.48	0.000106561	0.00407272	2.59527
S 11	35	16	166.075	0.315584	157.615	1100.	1.39486 ' 10 ⁻⁶	0.00813651	-0.803417
S 11	35	17	128.445	0.273305	202.594	1000.	3.10776 ' 10 ⁻⁶	0.00580361	-2.33054
S 11	35	18	105.065	0.189332	305.163	916.653	0.0000174169	0.00646898	-2.61049
S 11	35	19	64.7745	0.0207554	299.697	529.296	0.0000495524	0.00366251	1.95121
S 11	35	20	63.9271	0.299715	467.287	904.233	-9.96518 ' 10 ⁻⁶	0.00338014	-2.50179

Sample 11 Scan 36:

S	T	M	LL	w	s	t	a	% erg	f
S 11 36 1	716.607	0.0265744	223.215	1023.19	0.0000640822		0.511593	0.103455	
S 11 36 2	149.005	0.00701889	511.347	1579.35	-1.86153' 10 ⁻⁶		0.0675084	-0.451186	
S 11 36 3	320.876	0.0939401	67.9488	837.617	0.0000474029		0.115266	2.95548	
S 11 36 4	564.769	0.182487	60.5713	900.409	-0.0000144811		0.106386	1.06353	
S 11 36 5	98.0974	0.0975777	232.513	1000.01	1.2207755367319256' 10 ⁻⁶		0.0131788	-2.51302	
S 11 36 6	105.573	0.0579071	145.088	558.466	-5.13192' 10 ⁻⁷		0.0184147	2.50076	
S 11 36 7	74.9528	0.0981132	103.829	1690.18	9.96514' 10 ⁻⁶		0.0120369	-1.43008	
S 11 36 8	59.0538	0.0257733	704.354	951.634	-1.88915' 10 ⁻⁶		0.0088682	-2.45397	
S 11 36 9	107.104	0.113343	282.807	1077.39	6.31375' 10 ⁻⁶		0.0148066	2.9223	
S 11 36 10	45.9625	0.0879341	564.663	1013.98	-2.0951526983891363' 10 ⁻⁶		0.00588364	0.80924	
S 11 36 11	124.754	0.195104	332.536	1414.45	0.0000163752		0.0146713	2.93066	
S 11 36 12	107.566	0.0461881	462.204	1128.4	-0.0000156368		0.0112608	-0.119712	
S 11 36 13	166.279	0.144478	165.375	900.	2.9450267148168505' 10 ⁻⁶		0.0123966	-0.0193639	
S 11 36 14	52.8053	0.0163624	755.313	1273.88	-2.98217' 10 ⁻⁶		0.00446262	-2.61309	
S 11 36 15	161.088	0.235906	59.716	1200.	1.1747013680521735' 10 ⁻⁶		0.0116941	1.79111	
S 11 36 16	173.495	0.31616	158.439	1100.08	2.0397709396104935' 10 ⁻⁷		0.00768742	-0.820864	
S 11 36 17	127.895	0.17649	198.71	1200.	-1.26052' 10 ⁻⁶		0.00707961	1.83287	
S 11 36 18	111.056	0.274436	252.435	1000.31	0.		0.00453267	-2.14486	
S 11 36 19	69.7896	0.298856	430.788	879.022	-0.0000110754		0.00345849	-1.13901	
S 11 36 20	33.2366	0.134726	88.2713	1803.41	0.000114476		0.00156413	2.21572	

Sample 11 Scan 37:

S	T	M	LL	w	s	t	a	% erg	f
S 11 37 1	722.614	0.0265213	223.653	1023.25	0.0000640806			0.514518	0.0955883
S 11 37 2	151.914	0.00699128	515.281	1576.3	-1.8891478129560046	' 10 ⁻⁶		0.068316	-0.42933
S 11 37 3	199.806	0.104036	257.53	952.067	-0.0000253055			0.0753015	-2.35047
S 11 37 4	131.633	0.0862638	259.793	1011.85	-3.6306634326940763	' 10 ⁻⁶		0.0368874	1.11435
S 11 37 5	451.93	0.178792	112.249	888.603	-0.0000212685			0.0783321	-3.12904
S 11 37 6	176.141	0.0673663	405.344	761.386	-0.0000149254			0.0364477	2.12012
S 11 37 7	110.314	0.194034	823.565	1457.76	0.0000163893			0.019765	0.768996
S 11 37 8	280.404	0.144864	115.827	899.934	2.0014153373665129	' 10 ⁻⁷		0.0324164	0.360306
S 11 37 9	69.3961	0.0258239	704.981	954.269	-1.8316396499319585	' 10 ⁻⁶		0.00918845	-2.53569
S 11 37 10	93.7619	0.114667	575.279	930.987	-0.0000117828			0.0114439	-1.64168
S 11 37 11	82.2307	0.174166	248.384	1143.29	-7.76571	' 10 ⁻⁶		0.00918979	-0.790473
S 11 37 12	106.813	0.0462758	463.209	1134.12	-0.0000183354			0.0108632	-0.242434
S 11 37 13	48.1211	0.0163164	739.485	1267.52	-2.98699	' 10 ⁻⁶		0.00452749	-2.51455
S 11 37 14	137.544	0.233418	83.1665	1199.77	-3.13609	' 10 ⁻⁶		0.0110082	1.84511
S 11 37 15	145.857	0.316202	188.487	1100.	4.15504	' 10 ⁻⁶		0.00782968	-0.884831
S 11 37 16	197.274	0.0993348	129.578	1679.71	0.0000287147			0.0130699	-0.490075
S 11 37 17	101.494	0.192514	199.603	775.146	-0.0000167047			0.00487065	1.11266
S 11 37 18	64.5871	0.299192	449.082	877.915	-0.000010806			0.00344384	-0.967731
S 11 37 19	50.7779	0.21909	294.717	1002.58	0.0000434813			0.00255557	-2.62126
S 11 37 20	118.1	0.273527	212.961	1000.	2.15635	' 10 ⁻⁶		0.00449724	-2.05321

Sample 11 Scan 38:

S	T	M	LL	w	s	t	a	% erg	f
S 11 38 1	734.293	0.0228507	237.419	1046.88	0.0000654992			0.520155	-0.483392
S 11 38 2	147.035	0.00697561	547.525	1576.18	-2.27256 ' 10 ⁻⁶			0.0655505	-0.390026
S 11 38 3	203.2	0.102822	247.493	935.019	-0.000028336			0.0756322	-0.536349
S 11 38 4	262.214	0.179347	171.815	894.373	-0.0000232313			0.06587	2.01549
S 11 38 5	261.773	0.0866107	229.109	1002.63	-0.0000311422			0.0487039	2.34531
S 11 38 6	88.3158	0.06393	366.519	668.619	-0.0000144832			0.0188982	1.96904
S 11 38 7	108.33	0.193976	837.442	1471.94	0.0000156514			0.0210136	-1.91721
S 11 38 8	263.016	0.146484	115.197	899.997	-1.1978812205940977 ' 10 ⁻⁶			0.0342846	0.429088
S 11 38 9	89.0013	0.103182	354.346	1625.3	0.0000256976			0.0127202	-1.27784
S 11 38 10	82.7555	0.171931	251.688	1132.09	-0.0000102966			0.0108524	0.851518
S 11 38 11	66.4946	0.0486024	592.914	1055.6	1.1236737449130198 ' 10 ⁻⁶			0.0080932	2.96969
S 11 38 12	74.3595	0.0246585	362.391	880.373	0.0000139261			0.00843536	-1.20205
S 11 38 13	100.595	0.195076	200.455	800.	0.			0.00939297	1.91435
S 11 38 14	107.627	0.111615	338.596	810.635	-0.0000137166			0.0101916	-0.494165
S 11 38 15	141.015	0.233978	84.5543	1200.	1.2391385542960395 ' 10 ⁻⁶			0.0116448	1.68512
S 11 38 16	135.071	0.316169	163.253	1100.13	3.95042 ' 10 ⁻⁶			0.00763503	-1.00046
S 11 38 17	70.7625	0.0271689	380.03	1476.1	0.0000174204			0.00481019	1.09713
S 11 38 18	71.5706	0.0613349	254.916	1354.22	3.6626518917024992 ' 10 ⁻⁶			0.00453071	1.24455
S 11 38 19	71.4457	0.0835189	269.914	1533.35	3.38778 ' 10 ⁻⁷			0.00421068	-0.543305
S 11 38 20	119.959	0.273526	220.492	999.998	3.1348 ' 10 ⁻⁶			0.00507335	-2.12473

Sample 11 Scan 39:

S	T	M	LL	w	s	t	a	% erg	f
S 11	39	1	735.261	0.0228147	237.696	1047.1	0.0000654842	0.52062	-0.489041
S 11	39	2	149.097	0.00698697	547.597	1577.87	-2.2553609403381866' 10 ⁻⁶	0.0663379	-0.404361
S 11	39	3	334.608	0.0932744	67.4782	841.424	0.000104332	0.117313	2.47604
S 11	39	4	612.903	0.181517	52.366	903.186	-0.0000332612	0.102375	0.429584
S 11	39	5	105.875	0.0984786	221.467	1000.	3.0563844370792317' 10 ⁻⁶	0.0137757	-2.46154
S 11	39	6	113.97	0.0597087	150.745	560.079	1.3747' 10 ⁻⁶	0.0192695	2.38769
S 11	39	7	116.849	0.099742	976.482	1667.63	-0.000176485	0.0176216	1.13971
S 11	39	8	56.8721	0.178783	542.604	1256.4	-6.41278' 10 ⁻⁷	0.00785851	-1.95275
S 11	39	9	107.722	0.195435	303.197	1337.15	4.12653' 10 ⁻⁶	0.0137137	-0.576224
S 11	39	10	76.8216	0.0236912	562.162	901.191	6.60753' 10 ⁻⁶	0.00891576	-1.46701
S 11	39	11	128.063	0.111396	637.654	1239.85	7.72622' 10 ⁻⁶	0.0134215	-2.89854
S 11	39	12	50.2308	0.087725	1331.55	1457.4	-5.94398' 10 ⁻⁷	0.00481258	-0.323895
S 11	39	13	124.947	0.316509	158.301	1100.13	5.0542' 10 ⁻⁶	0.00837977	-0.977433
S 11	39	14	180.437	0.238023	83.242	1199.73	4.16871' 10 ⁻⁶	0.0137432	1.71841
S 11	39	15	115.905	0.0459762	585.672	1089.75	-0.0000199251	0.00780307	1.76255
S 11	39	16	57.7547	0.168283	605.879	1058.27	-3.3202180595181825' 10 ⁻⁶	0.00356335	0.941468
S 11	39	17	47.869	0.103496	757.316	926.915	2.0291207686787996' 10 ⁻⁶	0.00280137	0.874241
S 11	39	18	144.887	0.147176	193.595	900.	-9.2254' 10 ⁻⁸	0.00556229	-0.419107
S 11	39	19	62.9748	0.299707	428.605	909.698	-0.0000101433	0.00314745	2.07232
S 11	39	20	156.335	0.274708	194.959	1000.	3.2157139578611764' 10 ⁻⁶	0.00513769	-2.22754

Sample 11 Scan 40:

S	T	M	LL	w	s	t	a	% erg	f
S 11	40	1	743.156	0.0227492	237.726	1047.78	0.0000654649	0.52439	-0.498808
S 11	40	2	151.908	0.00701497	544.58	1577.72	-2.37197' 10 ⁻⁶	0.0669643	-0.399862
S 11	40	3	344.2	0.0931881	67.8402	841.584	0.0000968823	0.11885	2.4856
S 11	40	4	383.844	0.177396	147.34	910.293	-0.0000314099	0.0645616	-0.730786
S 11	40	5	90.9292	0.0984896	233.86	1000.	1.8327616993474376' 10 ⁻⁶	0.0141	-2.41997
S 11	40	6	95.1807	0.0596981	155.028	557.164	-2.5204122434616836' 10 ⁻⁷	0.0191211	2.57498
S 11	40	7	66.0648	0.0980296	88.2656	1666.64	-0.0000147398	0.0121717	0.914021
S 11	40	8	135.913	0.202715	552.947	1189.26	0.0000151015	0.0227878	-2.31591
S 11	40	9	336.228	0.147796	177.421	900.012	-2.25473' 10 ⁻⁶	0.0242415	0.400857
S 11	40	10	48.2912	0.0881454	667.909	1064.64	-1.3697942763373743' 10 ⁻⁶	0.00623649	2.58218
S 11	40	11	93.1354	0.11339	370.82	1092.74	7.20405' 10 ⁻⁶	0.0112096	1.11177
S 11	40	12	77.7034	0.0232375	542.809	890.753	8.12779' 10 ⁻⁶	0.00858563	-1.20338
S 11	40	13	129.814	0.19114	263.675	1001.1	0.000035694	0.0126619	-0.218015
S 11	40	14	103.262	0.0464756	452.277	1127.47	-0.0000177112	0.00918236	0.146461
S 11	40	15	136.81	0.233868	96.301	1200.	1.1987926845788253' 10 ⁻⁶	0.0105039	1.73752
S 11	40	16	162.251	0.316465	164.932	1100.	6.2730469969219315' 10 ⁻⁶	0.00797825	-0.893067
S 11	40	17	129.816	0.27342	209.322	1000.24	5.07431' 10 ⁻⁶	0.00633485	-2.1152
S 11	40	18	113.786	0.169089	227.687	1000.	-1.93273' 10 ⁻⁶	0.00596223	-1.85234
S 11	40	19	64.7044	0.301859	623.649	1020.96	-8.36721' 10 ⁻⁶	0.00336032	-0.0505713
S 11	40	20	87.5094	0.0245995	301.666	1551.34	0.0000116818	0.00421222	-0.67508

Sample 11 Scan 41:

S	T	M	LL	w	s	t	a	% erg	f
S 11	41	1	738.553	0.0227003	238.332	1047.92	0.0000655406	0.522195	-0.507191
S 11	41	2	151.311	0.00703514	540.487	1584.09	-2.3362534770440306' 10 ⁻⁶	0.0670293	-0.445904
S 11	41	3	497.711	0.0860382	97.7406	800.269	-2.2472943482185547' 10 ⁻⁶	0.0843622	-0.0157728
S 11	41	4	126.483	0.108026	447.406	977.087	-2.8502464562622107' 10 ⁻⁶	0.0387169	0.914867
S 11	41	5	457.737	0.179589	224.662	889.965	-0.000026556	0.056735	2.84455
S 11	41	6	139.33	0.0748274	646.46	847.306	-0.0000221509	0.0299681	1.51711
S 11	41	7	48.0921	0.0484642	597.19	1030.	6.95322' 10 ⁻⁷	0.00941194	-2.0641
S 11	41	8	118.538	0.205062	265.04	999.989	-0.0000235572	0.0211779	-0.311181
S 11	41	9	274.526	0.158488	137.043	1000.	-1.81554' 10 ⁻⁶	0.0282701	-2.2988
S 11	41	10	87.4357	0.0860317	486.213	1572.81	-0.0000402228	0.0118542	-2.97351
S 11	41	11	157.775	0.13816	208.325	1000.	-1.93821' 10 ⁻⁶	0.0127767	-0.744701
S 11	41	12	73.3711	0.0232293	639.685	885.137	7.34767' 10 ⁻⁶	0.00827416	-0.982874
S 11	41	13	81.0056	0.192975	207.692	1490.32	0.0000218074	0.0084569	0.770335
S 11	41	14	42.2026	0.037838	3208.66	827.943	6.52213' 10 ⁻⁶	0.00414185	-1.44517
S 11	41	15	79.0094	0.0784388	387.25	701.648	-0.0000233087	0.00729943	-1.84633
S 11	41	16	141.96	0.316725	189.31	1100.	-1.6591929722383039' 10 ⁻⁶	0.00832571	-0.873611
S 11	41	17	114.027	0.234711	138.402	1200.	3.1105953673363565' 10 ⁻⁶	0.00799381	1.86612
S 11	41	18	61.7578	0.21793	384.36	963.031	-5.3007' 10 ⁻⁶	0.00433992	-0.249251
S 11	41	19	144.897	0.273203	195.08	1000.01	5.06829' 10 ⁻⁶	0.00735787	-2.09383
S 11	41	20	62.155	0.125678	339.577	814.548	-6.70986' 10 ⁻⁶	0.00366204	-0.384425

Sample 11 Scan 42:

S	T	M	LL	w	s	t	a	% erg	f
S 11	42	1	745.984	0.0224934	239.267	1049.63	0.000065505	0.525732	-0.538678
S 11	42	2	157.02	0.00706959	536.854	1588.61	-2.30437' 10 ⁻⁶	0.0688489	-0.48205
S 11	42	3	350.595	0.0935283	67.4742	841.777	0.000100737	0.119727	2.47563
S 11	42	4	329.949	0.176302	222.108	887.387	-0.0000340166	0.0544286	-2.90114
S 11	42	5	92.0959	0.0986228	232.139	1000.	5.30606' 10 ⁻⁷	0.0139564	-2.40078
S 11	42	6	94.4063	0.0599504	156.729	556.757	7.10042' 10 ⁻⁷	0.0195223	2.60785
S 11	42	7	177.925	0.196226	216.824	871.432	-0.0000206452	0.0201038	0.459721
S 11	42	8	75.0358	0.0996933	79.5999	1683.97	-0.0000296749	0.0127938	-0.723678
S 11	42	9	304.432	0.151855	173.659	900.	-1.1269291118004927' 10 ⁻⁶	0.0316308	0.579341
S 11	42	10	93.9147	0.113545	363.65	1107.76	5.9336' 10 ⁻⁶	0.0118942	-0.494922
S 11	42	11	56.9441	0.0879417	581.856	1011.34	-1.6035017419140223' 10 ⁻⁶	0.00668636	1.07537
S 11	42	12	125.465	0.0387585	581.353	928.706	-0.0000199004	0.0134549	2.56121
S 11	42	13	89.3024	0.176265	584.997	1271.14	-0.0000102977	0.00859879	1.83807
S 11	42	14	69.0349	0.0190413	1132.99	1465.71	-5.55016' 10 ⁻⁶	0.00614048	1.02587
S 11	42	15	95.5592	0.194554	212.441	1365.94	1.3624041708287266' 10 ⁻⁶	0.00782618	0.252601
S 11	42	16	181.386	0.316609	167.028	1100.	3.2440167545013514' 10 ⁻⁶	0.0084669	-0.755316
S 11	42	17	136.359	0.233618	211.187	1200.	-6.23796' 10 ⁻⁹	0.00851823	1.86835
S 11	42	18	149.927	0.27319	196.227	1000.	8.27814' 10 ⁻⁶	0.00721011	-2.00807
S 11	42	19	86.4759	0.0381286	1005.3	1521.38	-0.0000114946	0.00446128	-0.932336
S 11	42	20	75.2532	0.213207	247.4	835.291	9.24949' 10 ⁻⁶	0.00358029	2.35541

Sample 11 Scan 43:

S	T	M	LL	w	s	t	a	% erg	f
S 11	43	1	985.546	0.0219293	240.028	1057.86	0.0000648888	0.626765	-0.61364
S 11	43	2	259.436	0.00708724	538.647	1590.57	-2.41939' 10 ⁻⁶	0.085151	-0.4595
S 11	43	3	431.258	0.086147	102.853	799.961	1.1818572839276466' 10 ⁻⁶	0.0716522	0.323995
S 11	43	4	159.562	0.107872	443.463	963.722	-2.81842' 10 ⁻⁶	0.0318144	2.73311
S 11	43	5	177.792	0.0685343	495.095	714.677	-0.0000225233	0.0299545	-1.16274
S 11	43	6	568.803	0.181141	56.7086	894.193	-0.0000220683	0.0483182	2.45508
S 11	43	7	86.8238	0.0483781	573.806	1056.52	5.40615' 10 ⁻⁸	0.00878416	-3.06086
S 11	43	8	112.733	0.0274036	227.027	680.115	-0.0000211085	0.0103246	-1.46001
S 11	43	9	139.399	0.0861201	388.59	1575.6	-0.0000363647	0.0112577	-2.99907
S 11	43	10	104.649	0.018572	640.464	1421.47	-5.56971' 10 ⁻⁶	0.00747786	1.99066
S 11	43	11	245.734	0.142162	140.968	899.999	-6.84966' 10 ⁻⁷	0.0115303	0.386252
S 11	43	12	114.005	0.194468	407.557	1311.58	4.62271' 10 ⁻⁶	0.00606075	-1.45908
S 11	43	13	138.907	0.0788291	470.334	709.899	-0.0000230544	0.00650908	-2.21964
S 11	43	14	82.7933	0.031439	266.437	1282.75	-0.0000152661	0.00347076	1.47437
S 11	43	15	75.988	0.007856	2282.72	4556.39	8.14902' 10 ⁻⁶	0.00294222	-0.793519
S 11	43	16	184.594	0.235461	73.6538	1200.	-2.1214605283969312' 10 ⁻⁸	0.00504117	2.08989
S 11	43	17	127.678	0.172068	522.981	1123.7	-0.0000130815	0.0038627	3.03198
S 11	43	18	205.354	0.316753	141.054	1100.	-1.89594' 10 ⁻⁶	0.0032476	-0.425505
S 11	43	19	116.577	0.274305	201.795	1000.	3.75249' 10 ⁻⁶	0.00270098	-1.72376
S 11	43	20	95.0224	0.128017	69.3732	1700.	-1.93568' 10 ⁻⁶	0.00163858	-2.0828

Sample 11 Scan 44:

S	T	M	LL	w	s	t	a	% erg	f
S 11	44	1	1318.37	0.0261041	220.516	1038.69	0.0000602951	0.732428	0.0800918
S 11	44	2	626.604	0.00715781	472.809	1585.71	-1.4800687137687586' 10 ⁻⁶	0.123839	-0.438238
S 11	44	3	100.91	0.0247449	94.6566	1165.09	0.0000157019	0.0135709	-1.183
S 11	44	4	467.609	0.0854007	118.976	809.562	-0.000432205	0.0477329	0.477079
S 11	44	5	88.3825	0.0870063	711.091	1117.58	-1.1746922219902008' 10 ⁻⁶	0.00674329	-1.09349
S 11	44	6	295.471	-0.0039788	259.988	705.586	0.000228525	0.0186063	1.56676
S 11	44	7	132.583	0.0598593	139.943	1322.03	5.15447' 10 ⁻⁶	0.00408428	-2.49798
S 11	44	8	80.9025	0.109625	490.035	1250.92	1.27354' 10 ⁻⁷	0.00386893	3.10035
S 11	44	9	122.581	0.0495476	1072.59	1032.49	6.31697' 10 ⁻⁶	0.00529689	-2.96425
S 11	44	10	102.471	0.0281375	387.306	695.824	-0.0000179126	0.00395591	-1.67769
S 11	44	11	117.551	0.182696	442.817	973.681	-0.0000239506	0.00406582	0.764646
S 11	44	12	97.9554	0.0983936	557.394	1455.59	1.8298657744371995' 10 ⁻⁷	0.00304142	-2.51828
S 11	44	13	70.6757	0.0742861	203.289	1000.	-8.8077' 10 ⁻⁶	0.00186308	-1.86542
S 11	44	14	164.397	0.0231788	271.652	1709.31	0.0000162824	0.00419768	2.23685
S 11	44	15	85.2869	0.13249	110.068	900.	-6.9140347534115065' 10 ⁻⁹	0.00152787	-0.688865
S 11	44	16	135.344	0.0667948	33.2886	444.814	-0.000231543	0.00278019	-2.62189
S 11	44	17	96.6208	0.197224	227.765	865.445	-0.0000190431	0.00163423	1.85822
S 11	44	18	125.893	0.171472	621.863	1144.08	-0.0000137914	0.0020743	-0.727592
S 11	44	19	68.6871	0.00971793	707.608	1022.63	0.0000123566	0.00102634	2.1779
S 11	44	20	186.381	0.316644	136.576	1100.13	1.0574099120895902' 10 ⁻⁷	0.00142187	-0.508529

Sample 11 Scan 45:

S	T	M	LL	w	s	t	a	% erg	f
S 11 45 1	1460.89	0.0194523	241.356	1087.33	0.0000627829			0.767969	-0.937311
S 11 45 2	733.897	0.00712431	541.753	1595.79	-2.62704' 10 ⁻⁶			0.120177	-0.412549
S 11 45 3	137.05	0.0330973	528.344	839.255	-0.0000244942			0.0141915	0.507944
S 11 45 4	363.753	0.0873364	66.1623	830.879	0.0000233558			0.0294607	-1.87814
S 11 45 5	201.818	0.0567989	144.71	549.517	-7.28833' 10 ⁻⁶			0.0122439	-2.36335
S 11 45 6	197.315	0.0246982	354.399	1534.54	0.0000104958			0.00983219	0.162477
S 11 45 7	88.7271	0.0176936	252.837	1125.49	6.74409' 10 ⁻⁶			0.00382699	0.485188
S 11 45 8	779.324	0.176284	47.8445	891.619	-0.0000247051			0.0115626	2.8756
S 11 45 9	100.296	0.097848	767.655	1317.71	-1.8863454849167582' 10 ⁻⁶			0.00283276	-1.27438
S 11 45 10	154.257	0.0434836	799.347	1625.97	3.0816057759729623' 10 ⁻⁶			0.00383836	1.58927
S 11 45 11	103.043	0.0879408	583.55	1373.34	7.72286' 10 ⁻⁷			0.00225309	1.86616
S 11 45 12	145.234	0.111165	380.807	1183.64	6.63658' 10 ⁻⁶			0.0028061	-2.20978
S 11 45 13	98.6825	0.193784	339.655	1244.48	-5.28675' 10 ⁻⁶			0.00168696	-0.73549
S 11 45 14	94.2973	0.00874313	819.548	199.588	-0.0000360584			0.00146367	-2.81883
S 11 45 15	108.365	0.0599589	586.647	1345.04	5.29201' 10 ⁻⁶			0.00151225	3.13145
S 11 45 16	173.435	0.143585	156.191	900.	5.07431' 10 ⁻⁶			0.00161701	-0.0540604
S 11 45 17	60.6671	0.0771093	868.674	1417.98	-3.84909' 10 ⁻⁶			0.000682564	-3.06537
S 11 45 18	175.488	0.235276	78.8583	1200.	1.5473924158736936' 10 ⁻⁶			0.00141987	2.08311
S 11 45 19	229.791	0.316737	146.167	1100.	1.2131393732153834' 10 ⁻⁶			0.00108014	-0.432094
S 11 45 20	124.783	0.274362	199.921	1000.31	3.1163967730816747' 10 ⁻⁶			0.0009307	-1.81931

Sample 11 Scan 46:

S	T	M	LL	w	s	t	a	% erg	f
S 11 46 1	1458.6	0.0204601	337.941	1145.82	0.000028236			0.767439	-1.98212
S 11 46 2	301.433	0.00805971	1396.88	2260.38	2.30419' 10 ⁻⁶			0.0605204	0.102602
S 11 46 3	521.525	0.0489051	314.047	822.648	3.4039928710220665' 10 ⁻⁶			0.0696464	-3.01197
S 11 46 4	231.655	0.0320151	439.936	963.476	-4.22094' 10 ⁻⁶			0.0210366	1.9644
S 11 46 5	389.225	0.0887553	66.5632	840.801	0.0000995547			0.0260183	-2.97211
S 11 46 6	139.903	0.022043	636.668	1460.75	-9.3191' 10 ⁻⁷			0.00713876	1.70695
S 11 46 7	487.314	0.181083	87.7807	893.736	-0.0000171481			0.0114022	2.61645
S 11 46 8	80.3953	0.0977301	249.868	999.972	3.8298198142160266' 10 ⁻⁸			0.00264517	-1.80816
S 11 46 9	145.398	0.0598147	1345.57	1338.17	5.41906' 10 ⁻⁶			0.00453195	3.07019
S 11 46 10	120.12	0.0327424	24.2508	1697.92	-0.000630126			0.00327765	-1.55539
S 11 46 11	90.7379	0.000363583	298.425	1093.5	9.12603' 10 ⁻⁸			0.00222704	1.54586
S 11 46 12	121.344	0.0885528	351.451	739.037	-0.0000512738			0.0026674	1.51556
S 11 46 13	66.3093	0.0449246	917.277	1379.69	3.4849648323234904' 10 ⁻⁶			0.0013265	-0.30982
S 11 46 14	102.179	0.199377	501.251	1272.02	0.0000171244			0.00187937	0.0234106
S 11 46 15	87.7716	0.0836984	470.521	1385.79	0.0000186643			0.00146794	0.0820632
S 11 46 16	248.576	0.145833	154.798	900.	-1.2041383118079767' 10 ⁻⁶			0.00259852	0.74149
S 11 46 17	97.1823	0.109395	464.987	1387.19	0.0000104378			0.00124122	0.0963132
S 11 46 18	55.7139	0.0563697	1024.71	1065.61	2.44827' 10 ⁻⁶			0.000659037	-0.623651
S 11 46 19	125.793	0.176125	208.653	1199.91	3.21889' 10 ⁻⁶			0.00105095	2.14358
S 11 46 20	230.034	0.316667	138.859	1100.	2.49113' 10 ⁻⁸			0.00116197	-0.379469

Sample 11 Scan 47:

S	T	M	LL	w	s	t	a	% erg	f
S 11 47 1	1292.36	0.0261575	221.098	1037.6	0.0000607096			0.725379	0.0829885
S 11 47 2	597.577	0.00718629	469.588	1586.15	-1.4467416926655304	' 10 ⁻⁶		0.12285	-0.457059
S 11 47 3	427.106	0.102835	81.6148	835.348	-0.000476731			0.0519672	-1.91386
S 11 47 4	179.311	0.00712505	551.942	977.515	-0.0000344826			0.0159968	1.68961
S 11 47 5	236.021	0.0588374	114.973	564.835	6.22792	' 10 ⁻⁶		0.017089	2.792
S 11 47 6	119.828	0.0872155	679.635	1169.8	-5.3622	' 10 ⁻⁷		0.00724948	0.618324
S 11 47 7	173.425	0.0476831	390.987	1239.42	-0.0000581989			0.00906702	2.1404
S 11 47 8	169.753	0.110939	203.598	1099.78	-1.6077751730202666	' 10 ⁻⁸		0.00621916	1.07582
S 11 47 9	109.815	0.0806622	544.027	1191.4	-0.0000242853			0.00433266	2.31312
S 11 47 10	123.783	0.0247669	216.364	1723.79	-0.0000284023			0.00434597	2.3709
S 11 47 11	111.656	0.17991	324.003	917.588	-0.0000336387			0.0034841	-1.2369
S 11 47 12	357.68	0.131306	163.848	900.019	1.9914010644829957	' 10 ⁻⁶		0.00562948	-0.694493
S 11 47 13	148.051	0.0541855	82.4521	936.177	0.0000714317			0.0032841	2.40907
S 11 47 14	82.3381	0.0583867	1069.39	1707.46	5.86573	' 10 ⁻⁶		0.00162667	0.0170028
S 11 47 15	52.8973	0.190366	871.794	1364.09	2.6393266377721796	' 10 ⁻⁶		0.000976533	0.605006
S 11 47 16	27.9586	0.0214092	1013.06	2945.1	-8.44028	' 10 ⁻⁶		0.000495649	-1.98141
S 11 47 17	74.9642	0.207507	324.716	952.613	0.0000205077			0.00125958	2.6579
S 11 47 18	74.4274	0.0753166	1082.74	1482.48	4.3866638830371155	' 10 ⁻⁶		0.00116054	2.43213
S 11 47 19	156.296	0.31696	157.683	1100.	3.2427960596234064	' 10 ⁻⁶		0.00136839	-0.446962
S 11 47 20	92.6554	0.127613	1339.33	1943.13	-0.000024097			0.00120805	-0.86397

Sample 11 Scan 48:

S	T	M	LL	w	s	t	a	% erg	f
S 11	48	1	1099.11	0.0213107	240.702	1064.76	0.0000643691	0.666832	-0.696288
S 11	48	2	336.496	0.00712319	534.623	1589.57	-2.46076 ' 10 ⁻⁶	0.0950044	-0.445444
S 11	48	3	474.294	0.0908591	72.3927	845.298	0.0000970347	0.089649	2.6346
S 11	48	4	149.27	0.0586849	151.925	562.23	-3.95208 ' 10 ⁻⁶	0.0204678	2.67112
S 11	48	5	89.5645	0.0982904	213.589	1000.	-7.0781 ' 10 ⁻⁷	0.0100354	-1.86906
S 11	48	6	77.0378	0.0885515	87.4853	1679.17	-7.91645 ' 10 ⁻⁶	0.00868573	0.228937
S 11	48	7	147.302	0.0386383	525.589	933.176	-0.0000196264	0.0148653	2.63332
S 11	48	8	502.742	0.185625	84.7869	889.02	-0.000038033	0.0250026	-2.64773
S 11	48	9	101.193	0.0326417	893.938	1441.35	-0.0000679132	0.00660831	2.59739
S 11	48	10	125.446	0.112305	560.889	1173.43	6.5633412251783735 ' 10 ⁻⁶	0.00729668	-1.21516
S 11	48	11	306.096	0.14726	128.237	899.917	-9.25058 ' 10 ⁻⁸	0.0109046	0.95012
S 11	48	12	166.809	0.0204105	320.308	1591.03	-0.0000207109	0.00671237	-1.00314
S 11	48	13	103.673	0.0881708	487.234	1026.58	-3.61217 ' 10 ⁻⁶	0.00363835	0.247064
S 11	48	14	133.121	0.19481	385.976	1237.23	7.29683 ' 10 ⁻⁷	0.00415138	0.851106
S 11	48	15	73.3011	0.0254822	468.705	941.623	-7.71384 ' 10 ⁻⁷	0.00206067	-1.93708
S 11	48	16	73.7643	0.0442013	1022.38	1551.02	1.4005692063530654 ' 10 ⁻⁶	0.00192668	-1.60196
S 11	48	17	92.7485	0.168046	229.192	1100.	-1.9448479257040374 ' 10 ⁻⁶	0.00159319	0.725551
S 11	48	18	146.368	0.0690528	216.514	1371.74	-0.0000253132	0.00320988	0.774075
S 11	48	19	73.1397	0.181316	1007.94	1382.06	-4.08654 ' 10 ⁻⁶	0.00143629	1.66426
S 11	48	20	208.219	0.316886	149.822	1100.	6.2678 ' 10 ⁻⁶	0.00191023	-0.353354

Sample 11 Scan 49:

S	T	M	LL	w	s	t	a	% erg	f
S 11	49	1	932.722	0.0263339	228.123	1027.91	0.0000638791	0.606519	0.0757232
S 11	49	2	263.46	0.00717442	482.302	1584.69	-1.6531736594478307 ' 10 ⁻⁶	0.0909112	-0.497083
S 11	49	3	484.926	0.0867459	111.129	825.496	-0.000530788	0.115742	-1.32101
S 11	49	4	215.3	0.0519884	348.739	714.514	7.91022 ' 10 ⁻⁶	0.0359182	0.859166
S 11	49	5	131.834	0.086798	728.018	1096.87	-9.98621 ' 10 ⁻⁷	0.0184669	0.159086
S 11	49	6	299.852	0.108875	233.871	1100.	1.7683970019501512 ' 10 ⁻⁹	0.0200455	0.58045
S 11	49	7	69.7135	0.0154613	770.067	1156.64	-2.5182259040249284 ' 10 ⁻⁶	0.00747467	-0.967795
S 11	49	8	124.039	0.179151	317.408	911.975	-0.0000342904	0.0120767	-0.363992
S 11	49	9	121.079	0.101339	264.114	1619.66	-3.61822 ' 10 ⁻⁷	0.0104285	-0.0210632
S 11	49	10	121.489	0.0266806	783.007	1086.42	-2.4325262605686826 ' 10 ⁻⁶	0.00926867	0.694302
S 11	49	11	303.454	0.132413	162.614	900.034	-1.6554311323758265 ' 10 ⁻⁶	0.0110378	-0.549488
S 11	49	12	142.066	0.0725421	620.089	930.021	-6.64885 ' 10 ⁻⁶	0.00804053	1.92393
S 11	49	13	147.127	0.0581466	180.211	1351.93	0.0000183344	0.00720411	1.37911
S 11	49	14	86.4503	0.192646	140.779	1453.6	-1.1689289975205547 ' 10 ⁻⁶	0.00261329	2.29701
S 11	49	15	117.467	0.246277	220.704	1100.	0.0000204879	0.00455736	1.36393
S 11	49	16	68.7092	0.221638	370.628	922.171	-0.0000102084	0.00254302	1.84696
S 11	49	17	143.029	0.174479	199.109	1200.	-2.6562151193154315 ' 10 ⁻⁹	0.0040349	2.01033
S 11	49	18	145.849	0.317074	159.71	1100.	3.87643 ' 10 ⁻⁶	0.00302306	-0.345802
S 11	49	19	65.6999	0.0593223	864.188	2187.37	-0.0000176402	0.00182475	-1.07178
S 11	49	20	59.6972	0.297484	438.696	819.313	-0.0000129307	0.00155719	-1.69469

Sample 11 Scan 50:

S	T	M	LL	w	s	t	a	% erg	f
S 11	50	1	778.079	0.021914	240.404	1054.59	0.0000652872	0.540713	-0.621781
S 11	50	2	176.785	0.00709924	536.24	1579.72	-2.34917 ' 10 ⁻⁶	0.0743431	-0.431407
S 11	50	3	286.868	0.0980501	217.776	880.092	-0.0000456116	0.0725999	-0.968927
S 11	50	4	122.471	0.0864266	187.618	950.97	-0.000017463	0.0260363	0.515536
S 11	50	5	426.155	0.179799	48.0884	929.799	-0.000020596	0.0762815	2.15029
S 11	50	6	189.946	0.0648711	200.311	613.744	-0.000022652	0.0362366	-0.804196
S 11	50	7	125.197	0.107896	173.113	800.	-1.94081 ' 10 ⁻⁶	0.0146901	0.520968
S 11	50	8	88.2816	0.0973212	109.502	1681.63	0.000010329	0.013396	-0.469202
S 11	50	9	124.645	0.201606	515.855	1169.45	0.0000170175	0.0170092	1.22021
S 11	50	10	69.7302	0.0264321	312.45	729.85	1.4956187801802379 ' 10 ⁻⁶	0.00863032	3.06747
S 11	50	11	117.93	0.168262	380.341	1014.54	-0.0000136878	0.0132936	2.44126
S 11	50	12	87.3559	0.0498899	370.364	1228.3	-0.0000170684	0.00888426	1.62634
S 11	50	13	87.7367	0.121808	537.395	1011.11	6.99256 ' 10 ⁻⁶	0.00817506	0.471413
S 11	50	14	75.7696	0.0181803	813.319	1386.4	-5.71543 ' 10 ⁻⁶	0.00650525	2.54158
S 11	50	15	143.937	0.316835	124.967	1000.	-1.87846 ' 10 ⁻⁶	0.0085432	-0.135298
S 11	50	16	110.522	0.224954	248.478	1093.34	-0.000041715	0.00770181	1.58517
S 11	50	17	81.5673	0.094155	633.529	1093.85	4.71592 ' 10 ⁻⁶	0.00520029	0.957818
S 11	50	18	124.095	0.273653	191.016	1000.13	5.0456 ' 10 ⁻⁶	0.00681236	-1.79239
S 11	50	19	158.675	0.141677	161.496	900.	-3.882 ' 10 ⁻⁶	0.00546511	0.69243
S 11	50	20	124.234	0.183035	244.497	1000.	-7.4225 ' 10 ⁻⁷	0.00394675	0.825447

Sample 11 Scan 51:

S	T	M	LL	w	s	t	a	% erg	f
S 11	51	1	742.459	0.0263359	228.057	1024.41	0.0000641495	0.524058	0.0754753
S 11	51	2	178.175	0.00712479	495.734	1575.34	-1.70824 ' 10 ⁻⁶	0.07755	-0.453232
S 11	51	3	219.555	0.099866	234.977	887.744	-0.0000323479	0.0781106	-1.9327
S 11	51	4	434.968	0.181379	68.8467	889.902	-0.0000293003	0.0845581	2.9013
S 11	51	5	312.265	0.0749341	365.652	828.375	-0.0000341977	0.0629508	-2.35933
S 11	51	6	62.7157	0.0259974	730.804	978.639	-1.613203500666588 ' 10 ⁻⁶	0.0104409	3.08562
S 11	51	7	160.172	0.113818	400.707	804.155	-0.000106538	0.0238748	0.302941
S 11	51	8	138.516	0.102769	1066.62	1615.96	0.0000278802	0.0177777	-0.428261
S 11	51	9	73.6078	0.194641	414.955	1213.36	-3.7811283425455805 ' 10 ⁻⁶	0.00849143	-1.05239
S 11	51	10	99.4582	0.0471954	496.047	1154.15	-0.0000192105	0.0105244	-1.15704
S 11	51	11	168.607	0.316884	259.339	1000.	-2.82781 ' 10 ⁻⁷	0.0082875	-0.314461
S 11	51	12	51.202	0.0162581	707.063	1249.71	-3.6868827225644264 ' 10 ⁻⁶	0.00460974	-2.25525
S 11	51	13	98.049	0.0835057	1317.19	1609.06	8.04764 ' 10 ⁻⁶	0.0081949	-0.653057
S 11	51	14	102.131	0.273686	185.665	1000.	5.0876721610238445 ' 10 ⁻⁶	0.0070927	-1.87427
S 11	51	15	139.507	0.245045	118.562	1200.	1.1978812205938682 ' 10 ⁻⁶	0.0092581	1.70937
S 11	51	16	68.5365	0.297036	182.484	691.995	-0.0000353456	0.00409498	-1.78579
S 11	51	17	99.2619	0.182003	926.054	1517.41	-0.000021932	0.0055849	2.69952
S 11	51	18	40.8747	0.330305	461.527	950.897	5.37923 ' 10 ⁻⁷	0.00214343	-2.32888
S 11	51	19	72.0722	0.0582532	728.829	855.214	-8.49488 ' 10 ⁻⁶	0.0035724	0.826137
S 11	51	20	49.8251	0.211457	337.329	822.44	7.86766 ' 10 ⁻⁶	0.00232339	-0.711225

Sample 11 Scan 52:

S	T	M	LL	w	s	t	a	% erg	f
S 11	52	1	749.831	0.0262505	230.141	1025.19	0.0000645305	0.527553	0.051488
S 11	52	2	178.896	0.00712586	498.142	1576.83	-1.8214949442558342 ' 10 ⁻⁶	0.0772586	-0.459423
S 11	52	3	229.633	0.0990752	231.836	855.14	-0.0000336708	0.0807983	1.31902
S 11	52	4	380.983	0.179603	43.9214	907.871	-0.0000338639	0.0990986	-0.367749
S 11	52	5	303.274	0.0705051	184.059	800.	-1.9377063231696275 ' 10 ⁻⁶	0.0373648	-0.709112
S 11	52	6	94.8242	0.0889926	258.122	1067.26	-8.26198 ' 10 ⁻⁶	0.0159504	2.67146
S 11	52	7	101.262	0.047438	708.849	876.887	0.0000177203	0.0154988	-2.04585
S 11	52	8	70.3719	0.107822	955.135	1315.95	8.06898 ' 10 ⁻⁷	0.00988277	1.42402
S 11	52	9	76.0371	0.0243214	488.779	916.657	7.7569 ' 10 ⁻⁶	0.00992494	-2.07632
S 11	52	10	76.7982	0.0585721	90.0486	1375.78	0.0000490502	0.00928683	-0.168814
S 11	52	11	103.366	0.195319	410.246	1300.71	8.13343 ' 10 ⁻⁶	0.0114251	0.332571
S 11	52	12	89.0602	0.0919456	180.835	1693.19	-0.0000105959	0.00893984	-1.55966
S 11	52	13	173.46	0.316645	122.008	999.989	3.5150352370483262 ' 10 ⁻⁶	0.00942359	-0.280618
S 11	52	14	121.486	0.169824	455.817	1044.29	-0.0000139825	0.00990128	-2.49227
S 11	52	15	135.011	0.141815	195.429	879.407	-0.0000361166	0.00625217	2.86909
S 11	52	16	114.065	0.27367	177.526	1000.	5.09035 ' 10 ⁻⁶	0.00687111	-1.89995
S 11	52	17	147.479	0.242006	212.441	1199.99	5.03451 ' 10 ⁻⁶	0.00828441	1.80094
S 11	52	18	74.8674	0.0477696	273.628	517.011	0.0000200897	0.00398491	-1.28171
S 11	52	19	83.7076	0.220049	650.457	1142.04	3.9570267130128065 ' 10 ⁻⁶	0.00411607	1.9507
S 11	52	20	79.1784	0.117932	654.484	1212.63	5.43462 ' 10 ⁻⁶	0.00358873	1.49616

Sample 11 Scan 53:

S	T	M	LL	w	s	t	a	% erg	f
S 11	53	1	751.63	0.0263529	228.04	1024.66	0.0000640079	0.528403	0.0801088
S 11	53	2	181.305	0.00713566	493.915	1576.78	-1.73481 ' 10 ⁻⁶	0.0780673	-0.45563
S 11	53	3	444.819	0.087215	131.785	824.698	-0.0000515821	0.14092	-1.52321
S 11	53	4	181.012	0.0518945	323.832	715.872	7.0324420559138465 ' 10 ⁻⁶	0.0416358	0.702985
S 11	53	5	104.741	0.0867037	713.116	1072.29	-1.13569 ' 10 ⁻⁶	0.0208657	2.04218
S 11	53	6	126.533	0.108985	238.585	1100.	-7.28601 ' 10 ⁻⁶	0.0223134	0.415626
S 11	53	7	159.888	0.179897	308.219	927.487	-0.0000339324	0.024624	2.79213
S 11	53	8	39.9746	0.0168411	375.646	695.215	0.0000183531	0.00556537	-1.57868
S 11	53	9	154.533	0.1319	154.656	900.	-1.0801901820395352 ' 10 ⁻⁷	0.0136624	-0.802361
S 11	53	10	59.7867	0.0283045	396.315	1211.88	-0.0000165296	0.00712527	-2.51835
S 11	53	11	98.8495	0.10121	240.834	1630.06	-7.21998 ' 10 ⁻⁷	0.0108852	-1.3315
S 11	53	12	55.8284	0.0740243	641.158	1050.21	-6.7704 ' 10 ⁻⁶	0.00568863	-0.854906
S 11	53	13	121.568	0.247027	213.048	1100.	-1.5394084021870257 ' 10 ⁻⁷	0.0110252	1.40063
S 11	53	14	106.307	0.191826	130.642	1497.85	-3.42126 ' 10 ⁻⁷	0.00501322	-0.273333
S 11	53	15	203.779	0.316642	124.12	999.966	-2.97873 ' 10 ⁻⁷	0.00859647	-0.0439971
S 11	53	16	118.457	0.222634	381.383	966.577	-0.0000136269	0.00831596	-1.80104
S 11	53	17	106.178	0.0573789	186.341	1338.49	2.3430481493254287 ' 10 ⁻⁶	0.00666056	2.16242
S 11	53	18	246.801	0.169871	163.777	1100.	-2.3957624411882476 ' 10 ⁻⁶	0.00768952	0.269261
S 11	53	19	124.881	0.203126	263.478	1000.	-0.0000216417	0.00511931	-0.515678
S 11	53	20	153.522	0.283493	332.411	866.9	0.0000284885	0.0066401	-2.46133

Sample 11 Scan 54:

S	T	M	LL	w	s	t	a	% erg	f
S 11	54	1	861.851	0.0216783	240.53	1057.56	0.0000652671	0.577621	-0.658007
S 11	54	2	211.794	0.00710888	535.407	1581.06	-2.3581299006704367 ' 10 ⁻⁶	0.0805161	-0.437725
S 11	54	3	395.011	0.0932511	69.0401	840.978	0.0000827303	0.111358	2.72327
S 11	54	4	80.1611	0.098061	252.	1000.	1.0592814440565459 ' 10 ⁻¹⁰	0.0123116	-2.29508
S 11	54	5	298.595	0.18729	259.716	1013.7	-0.0000287326	0.0338384	-0.617886
S 11	54	6	133.999	0.0574335	70.3434	570.364	0.000214024	0.0230425	1.59079
S 11	54	7	191.998	0.202293	235.378	1000.	1.9382135829540037 ' 10 ⁻⁶	0.0171723	-0.402777
S 11	54	8	83.0838	0.0888865	84.5822	1675.64	-0.0000184667	0.0114376	0.2596
S 11	54	9	243.98	0.164086	165.755	1000.	-1.92476 ' 10 ⁻⁶	0.0209751	-2.24233
S 11	54	10	107.808	0.0456579	666.689	1043.2	-8.04447 ' 10 ⁻⁶	0.0113496	-2.56519
S 11	54	11	133.123	0.145067	250.017	1000.	-3.2403864683855144 ' 10 ⁻⁷	0.0105295	-1.13234
S 11	54	12	126.42	0.111728	486.63	1206.94	7.3704 ' 10 ⁻⁶	0.0105898	0.937493
S 11	54	13	71.0969	0.0266163	915.849	1162.72	-9.88371 ' 10 ⁻⁷	0.00539307	-2.15988
S 11	54	14	88.2555	0.0179897	481.189	1370.67	-2.2847365244367076 ' 10 ⁻⁶	0.00618262	2.65295
S 11	54	15	73.3574	0.0895228	625.095	1082.17	8.46468 ' 10 ⁻⁷	0.00473955	1.24991
S 11	54	16	86.3041	0.0671538	391.001	1383.61	-0.00001991	0.00514863	-0.395085
S 11	54	17	129.711	0.232868	237.352	1106.89	-0.000031686	0.0068588	-0.940222
S 11	54	18	230.304	0.316603	121.876	1000.	-5.07877 ' 10 ⁻⁶	0.00588746	0.0206965
S 11	54	19	92.7215	0.192768	136.484	1509.03	0.0000476122	0.00392788	-2.44336
S 11	54	20	180.146	0.278414	366.853	950.268	0.0000319978	0.00666748	-0.717361

Sample 11 Scan 55:

S	T	M	LL	w	s	t	a	% erg	f
S 11	55	1	806.525	0.0261794	231.872	1027.14	0.0000647808	0.553593	0.027397
S 11	55	2	200.753	0.00714224	496.085	1581.07	-1.8872266166888401 ' 10 ⁻⁶	0.0810281	-0.483975
S 11	55	3	242.377	0.099246	229.232	861.322	-0.0000348007	0.0782547	0.81214
S 11	55	4	226.133	0.0699222	201.292	799.999	0.	0.035709	-0.663505
S 11	55	5	75.4473	0.088666	287.377	1059.31	-9.26436 ' 10 ⁻⁶	0.0181846	-2.73329
S 11	55	6	197.158	0.185166	267.395	998.927	-0.0000391699	0.0413796	2.34122
S 11	55	7	91.0021	0.0472727	713.591	881.833	0.0000177231	0.016585	-2.24349
S 11	55	8	126.028	0.202128	264.615	1030.52	-1.83845 ' 10 ⁻⁶	0.0205277	-0.198786
S 11	55	9	147.984	0.121017	767.132	1302.63	0.0000297802	0.0211219	-3.05534
S 11	55	10	83.2749	0.0242893	486.974	917.289	7.9329 ' 10 ⁻⁶	0.0105814	-2.07847
S 11	55	11	144.871	0.165311	268.827	1063.13	-0.0000197359	0.0164267	0.126308
S 11	55	12	156.169	0.124898	243.04	825.441	-0.0000657563	0.0152424	-1.95263
S 11	55	13	109.832	0.0579413	96.3146	1379.82	0.0000418564	0.00938001	-0.332227
S 11	55	14	89.734	0.216645	483.949	860.231	-0.0000314058	0.00693464	-2.22378
S 11	55	15	73.5583	0.106791	913.837	1445.65	0.000051824	0.00523833	2.35057
S 11	55	16	65.7208	0.105817	1277.62	1748.52	8.06462 ' 10 ⁻⁷	0.00436515	-0.404055
S 11	55	17	74.2471	0.190426	803.628	1322.71	3.4547123823931664 ' 10 ⁻⁶	0.00459836	1.846
S 11	55	18	179.138	0.316458	120.47	1000.	-1.9387073092477668 ' 10 ⁻⁶	0.00718578	-0.0404861
S 11	55	19	79.4673	0.0479988	284.499	508.546	0.0000213519	0.00400878	-0.858933
S 11	55	20	177.577	0.278138	346.175	950.462	0.0000335842	0.00788587	-0.854426

Sample 15 Scan 1:

S	T	M	LL	w	s	t	a	% erg	f
S 15	1	1	1798.52	0.0235159	238.082	1109.88	0.0000572022	0.834456	-0.152212
S 15	1	2	530.738	0.0061055	530.243	1529.1	-4.77031 ' 10 ⁻⁶	0.0677865	0.650407
S 15	1	3	904.121	0.0870276	240.281	954.07	-0.0000162572	0.0301109	-2.92659
S 15	1	4	221.09	0.0236119	803.575	964.914	-4.44141 ' 10 ⁻⁶	0.0131802	-1.50022
S 15	1	5	191.901	0.0717779	616.653	1083.02	-1.2125313617793825 ' 10 ⁻⁶	0.00930017	2.9218
S 15	1	6	143.98	0.0591956	738.699	958.397	-3.4431637017362693 ' 10 ⁻⁶	0.00589507	-0.925602
S 15	1	7	141.322	0.0398842	578.674	954.807	7.84228 ' 10 ⁻⁶	0.00501685	-2.20464
S 15	1	8	406.625	0.13619	156.707	900.004	-1.0000507344281825 ' 10 ⁻⁶	0.00755405	0.17532
S 15	1	9	130.333	0.0290658	297.8	550.654	-5.31929 ' 10 ⁻⁷	0.00311554	1.5298
S 15	1	10	108.834	0.0178834	341.585	1369.03	-2.0124729831846956 ' 10 ⁻⁷	0.00230789	-1.83951
S 15	1	11	122.747	0.098998	801.265	1026.94	-3.24482 ' 10 ⁻⁶	0.00231864	2.17684
S 15	1	12	285.377	0.118412	176.365	899.931	-9.96492 ' 10 ⁻⁷	0.00440251	-1.53629

Sample 15 Scan 2:

S	T	M	LL	w	s	t	a	% erg	f
S 15	2	1	1749.34	0.0230709	239.711	1111.59	0.0000581722	0.826112	-0.249982
S 15	2	2	527.75	0.00620521	536.865	1527.68	-5.19064 ' 10 ⁻⁶	0.0709566	0.641525
S 15	2	3	413.947	0.0862769	299.598	908.577	-0.0000254719	0.0345217	1.13817
S 15	2	4	231.855	0.023794	824.647	969.238	-4.31808 ' 10 ⁻⁶	0.0139318	-1.66912
S 15	2	5	126.708	0.059504	721.854	987.855	-3.15421 ' 10 ⁻⁶	0.0063534	-2.74384
S 15	2	6	237.764	0.073603	154.577	1200.	-1. ' 10 ⁻⁶	0.00740538	0.695322
S 15	2	7	146.405	0.0393275	183.675	666.627	-0.0000481224	0.00539691	-2.15771
S 15	2	8	410.427	0.136317	131.475	899.989	-1. ' 10 ⁻⁶	0.00760185	0.182215
S 15	2	9	94.9515	0.0179312	421.846	1376.57	-1.6568615269637439 ' 10 ⁻⁶	0.00241198	-1.92071
S 15	2	10	126.292	0.0352605	292.855	1163.78	-2.3505476408644155 ' 10 ⁻⁶	0.00287296	2.59502
S 15	2	11	435.407	0.11559	193.834	1018.52	7.88858 ' 10 ⁻⁶	0.00447359	-3.07149
S 15	2	12	145.891	0.096936	175.716	640.367	-2.70607 ' 10 ⁻⁷	0.00228948	2.09394

Sample 15 Scan 3:

S	T	M	LL	w	s	t	a	% erg	f
S 15	3	1	1700.53	0.0230669	239.927	1110.53	0.0000582876	0.817413	-0.252548
S 15	3	2	497.481	0.00619962	535.828	1525.8	-5.19019 ' 10 ⁻⁶	0.0712382	0.643393
S 15	3	3	682.488	0.0878379	185.839	961.554	-0.0000159593	0.0321423	2.57055
S 15	3	4	192.781	0.0719704	586.346	1025.37	-7.84263 ' 10 ⁻⁷	0.013701	0.652405
S 15	3	5	245.415	0.0238221	821.3	969.503	-4.2991 ' 10 ⁻⁶	0.0140233	-1.70154
S 15	3	6	148.641	0.0592331	755.282	966.285	-3.3608035519223875 ' 10 ⁻⁶	0.00696284	-1.5373
S 15	3	7	278.071	0.13657	156.71	900.	-1.0003193236954523 ' 10 ⁻⁶	0.00928255	0.167167
S 15	3	8	178.67	0.0407145	345.93	677.911	-0.0000259623	0.00559007	-2.8391
S 15	3	9	198.756	0.124401	247.244	1007.17	-8.0749 ' 10 ⁻⁶	0.00434486	-2.0191
S 15	3	10	111.542	0.0181411	910.21	1313.77	-1.1722147971495815 ' 10 ⁻⁶	0.00255744	-0.776037
S 15	3	11	129.288	0.0348794	246.024	1162.04	-7.77776 ' 10 ⁻⁶	0.00262812	2.71414
S 15	3	12	79.4873	0.227931	453.65	1193.19	8.84097 ' 10 ⁻⁶	0.00145501	3.02786

Sample 15 Scan 4:

S	T	M	LL	w	s	t	a	% erg	f
S 15	4	1	1757.57	0.0221669	242.072	1119.11	0.0000581589	0.827536	-0.401153
S 15	4	2	591.226	0.00638727	545.711	1540.56	-5.38122 ' 10 ⁻⁶	0.0765875	0.574241
S 15	4	3	175.144	0.023949	821.817	980.395	-4.2624436758733335 ' 10 ⁻⁶	0.0152276	-1.95944
S 15	4	4	418.386	0.0856583	314.841	891.344	-0.000026359	0.0271961	2.5805
S 15	4	5	110.376	0.0596052	722.594	1002.25	-3.3528 ' 10 ⁻⁶	0.00547068	2.75221
S 15	4	6	197.185	0.0737385	174.008	1200.	-1.0139150640813647 ' 10 ⁻⁶	0.00598628	0.689327
S 15	4	7	141.884	0.0370856	306.444	610.127	-0.000024775	0.00540925	-0.210961
S 15	4	8	318.869	0.136799	135.516	899.998	-1. ' 10 ⁻⁶	0.00804015	0.0173026
S 15	4	9	114.261	0.0183913	1002.2	1385.	-1.24372 ' 10 ⁻⁶	0.00296321	-2.00687
S 15	4	10	241.442	0.116013	356.158	865.322	-0.0000282145	0.00525021	2.64682
S 15	4	11	135.876	0.0345194	280.706	1169.6	-7.15664 ' 10 ⁻⁶	0.0024426	2.52613
S 15	4	12	95.2385	0.22838	444.959	1167.51	9.46802 ' 10 ⁻⁶	0.00152464	2.48629

Sample 15 Scan 5:

S	T	M	LL	w	s	t	a	% erg	f
S 15	5	1	1766.11	0.0220984	242.76	1120.33	0.0000578526	0.829002	-0.406534
S 15	5	2	606.026	0.00628586	539.629	1538.82	-5.06118 ' 10 ⁻⁶	0.0772926	0.582966
S 15	5	3	179.437	0.0239908	837.614	983.137	-4.20957 ' 10 ⁻⁶	0.0151962	-2.01075
S 15	5	4	417.037	0.0855775	315.505	890.735	-0.0000263667	0.0263633	2.66798
S 15	5	5	116.568	0.0596112	711.938	1003.02	-3.25515 ' 10 ⁻⁶	0.00560577	2.72256
S 15	5	6	223.227	0.0735968	196.416	1200.03	-1.0148066470096308 ' 10 ⁻⁶	0.00583878	0.728233
S 15	5	7	150.774	0.0370649	308.129	609.546	-0.0000250522	0.00552876	-0.161007
S 15	5	8	294.773	0.136792	105.72	900.	-1.0000000071900872 ' 10 ⁻⁶	0.00736092	0.0130619
S 15	5	9	123.2	0.0180753	958.093	1359.39	-9.24617 ' 10 ⁻⁷	0.00308484	-1.51357
S 15	5	10	113.146	0.0342857	288.83	1171.62	-7.16626 ' 10 ⁻⁶	0.00251676	2.46296
S 15	5	11	236.633	0.124054	206.218	1047.97	-8.99068 ' 10 ⁻⁶	0.0034781	-0.840373
S 15	5	12	130.237	0.0964105	162.743	640.534	4.88311 ' 10 ⁻⁶	0.00185651	1.97282

Sample 15 Scan 6:

S	T	M	LL	w	s	t	a	% erg	f
S 15	6	1	1861.59	0.0216169	242.902	1127.91	0.0000572091	0.844575	-0.472875
S 15	6	2	736.423	0.00624808	543.745	1544.99	-4.99205 ' 10 ⁻⁶	0.0804744	0.582969
S 15	6	3	241.146	0.0239747	831.665	986.938	-4.18687 ' 10 ⁻⁶	0.0157741	-2.03397
S 15	6	4	385.884	0.0848564	327.959	876.826	-0.0000270407	0.0185163	-2.24367
S 15	6	5	120.539	0.059744	701.668	1012.75	-3.24108 ' 10 ⁻⁶	0.00446507	2.3732
S 15	6	6	165.365	0.0408401	315.057	692.308	-0.0000589202	0.00531242	-2.92679
S 15	6	7	111.993	0.0176913	425.114	1430.09	-1.5740239002193555 ' 10 ⁻⁶	0.00312313	-2.66384
S 15	6	8	181.242	0.0714954	71.6286	1198.99	-0.000192777	0.00436867	1.40451
S 15	6	9	386.306	0.130117	234.812	1000.12	-1. ' 10 ⁻⁶	0.00481428	-0.708115
S 15	6	10	152.192	0.0500568	494.47	1196.57	0.000175443	0.00242418	1.47191
S 15	6	11	240.583	0.0478712	2259.89	961.789	-0.0000179086	0.00315253	-2.01881
S 15	6	12	80.9307	0.00949718	557.061	327.48	-0.0000352953	0.000900783	2.1978

Sample 15 Scan 7:

S	T	M	LL	w	s	t	a	% erg	f
S 15	7	1	1772.23	0.0225201	243.019	1117.71	0.0000570743	0.830046	-0.317408
S 15	7	2	596.505	0.00625899	538.955	1543.21	-4.93529 ' 10 ⁻⁶	0.0758985	0.578084
S 15	7	3	152.468	0.0283091	1541.16	1441.38	-4.79339 ' 10 ⁻⁶	0.0131157	-1.28033
S 15	7	4	405.453	0.0847998	261.53	869.478	-0.0000284847	0.0265398	-1.7026
S 15	7	5	137.711	0.0593579	709.83	961.155	-3.26875 ' 10 ⁻⁶	0.00682896	-1.04894
S 15	7	6	160.29	0.0407355	521.215	698.412	-0.0000553695	0.00685019	2.98521
S 15	7	7	142.084	0.0700687	437.98	1250.7	-4.83151 ' 10 ⁻⁶	0.00519409	-2.89959
S 15	7	8	96.7101	0.0181736	1059.82	1490.14	-1.8863068258770428 ' 10 ⁻⁶	0.00313608	2.41678
S 15	7	9	114.995	0.0318305	975.794	995.118	-5.44993 ' 10 ⁻⁶	0.00335464	2.03609
S 15	7	10	383.182	0.133023	243.255	1000.	-9.99989 ' 10 ⁻⁷	0.00656323	-0.708674
S 15	7	11	121.327	0.0941171	124.971	668.997	2.6482688693529817 ' 10 ⁻⁶	0.00204949	-0.589774
S 15	7	12	162.195	0.116943	213.426	1000.	-1.0000009788210643 ' 10 ⁻⁶	0.00233647	-0.594543

Sample 15 Scan 8:

S	T	M	LL	w	s	t	a	% erg	f
S 15	8	1	1616.45	0.0233463	242.585	1107.8	0.0000568971	0.801397	-0.169829
S 15	8	2	440.621	0.00624281	535.051	1540.53	-4.87808 ' 10 ⁻⁶	0.0704165	0.579929
S 15	8	3	422.533	0.0876575	223.252	962.008	-0.0000178359	0.0369095	2.46007
S 15	8	4	140.937	0.0719001	653.701	1089.72	-8.44046 ' 10 ⁻⁷	0.0118291	2.22725
S 15	8	5	185.317	0.0237038	829.229	967.36	-4.39622 ' 10 ⁻⁶	0.0132208	-1.63844
S 15	8	6	139.601	0.0590921	718.81	956.609	-3.0584546842334427 ' 10 ⁻⁶	0.00846002	-1.0618
S 15	8	7	530.916	0.132375	139.224	1000.	-1.0000000095038466 ' 10 ⁻⁶	0.0174284	-0.910285
S 15	8	8	151.201	0.0406881	342.908	672.629	-0.0000263307	0.00547849	-2.71784
S 15	8	9	123.219	0.102007	707.865	1317.84	0.0000149887	0.00389096	-3.11375
S 15	8	10	183.315	0.0241852	660.749	1217.17	0.0000562025	0.00496987	0.521388
S 15	8	11	152.12	0.229569	259.867	1000.	-9.99968 ' 10 ⁻⁷	0.00187655	-2.77274
S 15	8	12	240.001	0.150288	175.077	1050.57	0.0000649372	0.00443059	1.89009

Sample 15 Scan 9:

S	T	M	LL	w	s	t	a	% erg	f
S 15	9	1	1659.12	0.023192	242.681	1109.94	0.0000566479	0.809693	-0.193795
S 15	9	2	481.367	0.00626366	536.511	1545.29	-4.86722 ' 10 ⁻⁶	0.0722977	0.564583
S 15	9	3	346.216	0.0872685	247.38	954.248	-0.00001823	0.0334031	-3.0949
S 15	9	4	176.575	0.0237579	837.152	974.273	-4.4265605832329755 ' 10 ⁻⁶	0.0134701	-1.7808
S 15	9	5	151.779	0.071866	664.649	1123.21	-9.93652 ' 10 ⁻⁷	0.0098214	-0.117898
S 15	9	6	146.228	0.0590622	727.69	953.09	-3.0146434075988425 ' 10 ⁻⁶	0.00815173	-0.798196
S 15	9	7	111.291	0.0406202	354.267	671.193	-0.0000264277	0.00545248	-2.6429
S 15	9	8	244.387	0.13009	257.486	1000.	-9.84413 ' 10 ⁻⁷	0.00969229	-0.781929
S 15	9	9	114.909	0.0991983	775.776	1033.37	-2.42142 ' 10 ⁻⁶	0.00397577	1.17388
S 15	9	10	172.329	0.0112575	377.533	1335.12	0.000055962	0.00516834	-1.51445
S 15	9	11	300.68	0.146221	173.041	900.	-9.37278 ' 10 ⁻⁷	0.0056048	0.485008
S 15	9	12	210.285	0.117247	341.95	900.225	0.0000170163	0.00414188	-2.01323

Sample 15 Scan 10:

S	T	M	LL	w	s	t	a	% erg	f
S 15	10	1	1697.65	0.023142	243.198	1111.68	0.0000561775	0.816887	-0.192249
S 15	10	2	514.842	0.00624718	537.289	1548.69	-4.78122 ' 10 ⁻⁶	0.0732168	0.561628
S 15	10	3	359.652	0.0866243	284.307	906.	-0.0000274143	0.0327456	1.32869
S 15	10	4	198.782	0.0236943	841.748	971.408	-4.4476622943162605 ' 10 ⁻⁶	0.0136383	-1.68121
S 15	10	5	135.755	0.0592373	687.051	957.058	-3.0213460778474225 ' 10 ⁻⁶	0.00787182	-0.92734
S 15	10	6	127.993	0.074217	282.282	1210.07	6.92695 ' 10 ⁻⁶	0.00650423	-0.176254
S 15	10	7	126.309	0.0359006	330.822	590.583	-0.000024858	0.00565214	0.418681
S 15	10	8	545.849	0.127733	145.038	1000.	-1. ' 10 ⁻⁶	0.012397	-0.811367
S 15	10	9	154.776	0.0294584	88.7028	1212.36	0.0000409105	0.00424227	0.820247
S 15	10	10	97.0381	0.0966737	208.261	640.595	4.5180819268990305 ' 10 ⁻⁶	0.00234078	1.98208
S 15	10	11	81.3582	0.0154327	89.3299	1560.42	0.000078521	0.00179486	1.26199
S 15	10	12	205.673	0.150607	257.636	1000.	-1. ' 10 ⁻⁶	0.00328969	-2.02919

Sample 15 Scan 11:

S	T	M	LL	w	s	t	a	% erg	f
S 15	11	1	1587.39	0.023514	242.556	1105.9	0.0000562456	0.795542	-0.127489
S 15	11	2	419.977	0.00622246	536.702	1544.5	-4.80692 ' 10 ⁻⁶	0.0697357	0.574335
S 15	11	3	325.882	0.0878503	257.32	962.696	-0.0000189255	0.0366102	2.31952
S 15	11	4	110.872	0.0718382	683.394	1135.43	-1.0260671938065485 ' 10 ⁻⁶	0.0101468	-1.11059
S 15	11	5	161.888	0.02361	831.308	961.095	-4.41335 ' 10 ⁻⁶	0.0129344	-1.50176
S 15	11	6	125.945	0.0590099	725.038	948.681	-2.9422476099630805 ' 10 ⁻⁶	0.00870943	-0.638119
S 15	11	7	72.9105	0.0993524	753.37	1040.15	-1.8329653905201133 ' 10 ⁻⁶	0.00456277	0.222897
S 15	11	8	374.209	0.137636	136.353	900.026	-9.95853 ' 10 ⁻⁷	0.0140487	-0.107836
S 15	11	9	260.127	0.120936	232.862	996.221	-0.0000188108	0.00837976	-0.593252
S 15	11	10	163.743	0.0363052	342.819	593.622	-0.000025856	0.00572416	0.241738
S 15	11	11	144.095	0.0281828	145.443	1206.59	0.0000545846	0.00431756	0.799979
S 15	11	12	105.36	0.231355	461.011	1146.3	-0.0000105921	0.00278439	1.28529

Sample 15 Scan 12:

S	T	M	LL	w	s	t	a	% erg	f
S 15	12	1	1605.21	0.0235172	241.899	1106.54	0.0000561649	0.799153	-0.127435
S 15	12	2	435.754	0.00623464	538.057	1547.1	-4.80197 ' 10 ⁻⁶	0.0705428	0.56584
S 15	12	3	723.321	0.0877102	241.043	957.573	-0.0000188124	0.0354587	2.81678
S 15	12	4	117.267	0.0718778	683.693	1128.08	-9.1891 ' 10 ⁻⁷	0.0103334	-0.536816
S 15	12	5	170.315	0.0235511	822.661	956.323	-4.37182 ' 10 ⁻⁶	0.0130061	-1.3841
S 15	12	6	129.661	0.0589548	735.635	946.053	-2.9605330269058734 ' 10 ⁻⁶	0.00851752	-0.436255
S 15	12	7	294.688	0.138041	117.659	899.991	-1.0145592421540297 ' 10 ⁻⁶	0.0133416	-0.0745742
S 15	12	8	164.67	0.12331	233.29	952.302	-8.54794 ' 10 ⁻⁶	0.0070835	-1.75419
S 15	12	9	150.209	0.0362911	348.032	592.684	-0.0000260702	0.00573208	0.299835
S 15	12	10	114.576	0.0991806	773.294	1016.86	-2.16331 ' 10 ⁻⁶	0.00382862	2.68663
S 15	12	11	152.509	0.0288434	130.399	1206.	0.0000539239	0.00446098	0.836793
S 15	12	12	74.3171	0.112371	601.364	971.875	-7.36609 ' 10 ⁻⁶	0.00193812	2.61329

Sample 15 Scan 13:

S	T	M	LL	w	s	t	a	% erg	f
S 15	13	1	1595.55	0.0235466	242.051	1106.38	0.0000559883	0.797203	-0.117546
S 15	13	2	424.641	0.00620536	537.014	1545.63	-4.77931 ' 10 ⁻⁶	0.0697677	0.579111
S 15	13	3	310.605	0.0861083	261.432	925.476	-0.0000228492	0.0351184	-0.604832
S 15	13	4	145.083	0.0235454	826.821	956.894	-4.40999 ' 10 ⁻⁶	0.0130228	-1.39156
S 15	13	5	110.085	0.0589628	722.689	937.925	-2.9631303852241762 ' 10 ⁻⁶	0.00869395	0.0496483
S 15	13	6	120.521	0.0724526	547.648	1205.92	-1.3679984972579015 ' 10 ⁻⁷	0.00848243	0.148476
S 15	13	7	275.811	0.138378	124.35	900.	-9.37278 ' 10 ⁻⁷	0.0141136	-0.113119
S 15	13	8	198.68	0.11904	247.753	927.909	0.0000201012	0.00929782	0.85427
S 15	13	9	145.249	0.0360994	348.268	589.975	-0.0000259898	0.00578811	0.385896
S 15	13	10	130.079	0.0286389	133.984	1207.56	0.0000539251	0.00451613	0.79967
S 15	13	11	64.5145	0.0973229	412.391	1516.28	-0.0000239566	0.00203014	-2.98299
S 15	13	12	107.062	0.0967981	349.23	709.256	-8.0266 ' 10 ⁻⁷	0.00309301	1.50661

Sample 15 Scan 14:

S	T	M	LL	w	s	t	a	% erg	f
S 15	14	1	1855.58	0.0216469	242.109	1130.3	0.0000553052	0.843637	-0.437759
S 15	14	2	750.733	0.00620313	550.463	1559.36	-4.6324 ' 10 ⁻⁶	0.081835	0.547688
S 15	14	3	245.777	0.0236678	822.705	965.339	-4.10849 ' 10 ⁻⁶	0.0158569	-1.48293
S 15	14	4	293.538	0.0847815	324.426	863.706	-0.0000291712	0.0144757	-1.13601
S 15	14	5	95.8503	0.059427	713.03	982.44	-3.2896476719047168 ' 10 ⁻⁶	0.00387814	-1.96352
S 15	14	6	145.915	0.037366	162.505	644.672	-0.0000542464	0.00523418	-1.13415
S 15	14	7	105.54	0.0172677	429.273	1473.82	-1.8904736309608843 ' 10 ⁻⁶	0.00333694	2.96216
S 15	14	8	114.107	0.0340157	379.217	1210.73	-7.7321 ' 10 ⁻⁷	0.00323284	1.2048
S 15	14	9	132.473	0.0729767	141.283	1200.	-1. ' 10 ⁻⁶	0.00284288	0.905232
S 15	14	10	287.184	0.139079	117.928	900.	-1.0067450197803672 ' 10 ⁻⁶	0.00568569	-0.00118103
S 15	14	11	207.983	0.119033	226.77	974.246	-0.0000194914	0.00291336	2.15424
S 15	14	12	89.7873	0.232739	477.033	1192.41	-9.42253 ' 10 ⁻⁶	0.00131422	3.11008

Sample 15 Scan 15:

S	T	M	LL	w	s	t	a	% erg	f
S 15	15	1	1856.01	0.0222672	241.516	1125.07	0.0000550123	0.843704	-0.326671
S 15	15	2	715.116	0.00618075	549.033	1560.48	-4.60352 ' 10 ⁻⁶	0.0791299	0.551903
S 15	15	3	196.475	0.0281768	1568.27	1430.86	-4.90941 ' 10 ⁻⁶	0.013439	-0.817157
S 15	15	4	298.996	0.0845263	327.891	864.739	-0.0000285745	0.0159944	-1.16319
S 15	15	5	211.746	0.0280079	170.535	600.652	-0.000131265	0.00875798	0.618219
S 15	15	6	122.614	0.0248471	3962.22	4065.85	-1.3989115137416466 ' 10 ⁻⁶	0.0042823	-1.94018
S 15	15	7	130.453	0.0719938	589.735	1211.71	-1.1025474640506084 ' 10 ⁻⁶	0.00401385	0.243097
S 15	15	8	110.213	0.0597531	427.945	1337.11	4.12063 ' 10 ⁻⁶	0.00300602	1.31618
S 15	15	9	130.149	0.0347138	316.201	1113.75	-5.05731 ' 10 ⁻⁶	0.00314843	-1.51025
S 15	15	10	36.5828	0.0000362336	228.493	300.237	-1.3828801862349654 ' 10 ⁻⁸	0.000813656	-1.62221
S 15	15	11	304.161	0.138732	113.299	900.	-9.76043 ' 10 ⁻⁷	0.0052202	0.0937375
S 15	15	12	154.72	0.123289	262.819	1031.47	-9.7311 ' 10 ⁻⁶	0.00234327	1.37624

Sample 15 Scan 16:

S	T	M	LL	w	s	t	a	% erg	f
S 15	16	1	1845.23	0.0243871	227.393	1111.3	0.0000523781	0.84201	0.0419662
S 15	16	2	813.15	0.00635757	495.498	1559.35	-4.82387 ' 10 ⁻⁶	0.0867951	0.576537
S 15	16	3	255.624	0.0230255	439.526	756.506	3.6047811254304404 ' 10 ⁻⁶	0.015441	2.88079
S 15	16	4	190.137	0.0367974	842.758	1138.81	0.0000124677	0.00917946	2.54992
S 15	16	5	315.407	0.0850567	334.658	871.214	-0.0000270319	0.0118566	-1.76431
S 15	16	6	105.605	0.0602516	737.733	1073.39	-3.5329 ' 10 ⁻⁹	0.00320446	-1.41283
S 15	16	7	70.9751	0.0126007	575.869	857.712	2.7502610911447907 ' 10 ⁻⁶	0.00197116	-3.12062
S 15	16	8	57.4746	-5.33514	101899.	-205742.	-0.0000129451	0.00128632	-1.9848
S 15	16	9	115.375	0.0731278	442.887	1298.24	4.70356 ' 10 ⁻⁶	0.00273813	-0.0489722
S 15	16	10	259.652	0.125314	255.492	999.992	-1.0098180964373598 ' 10 ⁻⁶	0.00366865	-0.866498
S 15	16	11	213.154	0.141568	193.182	900.	-1. ' 10 ⁻⁶	0.00278254	0.316182
S 15	16	12	88.808	0.232724	471.239	1197.26	-8.85599 ' 10 ⁻⁶	0.00135443	2.01477

Sample 15 Scan 17:

S	T	M	LL	w	s	t	a	% erg	f
S 15	17	1	1889.35	0.0212639	240.969	1136.61	0.0000545178	0.84883	-0.490957
S 15	17	2	826.69	0.00614734	554.053	1562.78	-4.51465 ' 10 ⁻⁶	0.0841718	0.556647
S 15	17	3	135.809	0.0273895	221.709	1527.97	0.0000183226	0.00825876	2.56341
S 15	17	4	338.265	0.0228937	373.006	730.044	4.50886 ' 10 ⁻⁶	0.0162943	-2.7258
S 15	17	5	297.322	0.0827484	316.079	817.086	-0.0000314426	0.0104116	2.89063
S 15	17	6	213.997	0.0611241	478.426	874.79	-0.000031236	0.00579291	-0.89311
S 15	17	7	130.673	-0.773146	84711.4	-14254.2	-0.0000265253	0.00269293	0.29315
S 15	17	8	231.38	0.123572	223.178	1000.	-1. ' 10 ⁻⁶	0.0035854	-0.856643
S 15	17	9	61.2238	0.0949218	542.202	860.095	2.25526 ' 10 ⁻⁶	0.00104015	0.0948512
S 15	17	10	298.022	0.142307	169.214	900.	-9.76041 ' 10 ⁻⁷	0.00291055	0.244028
S 15	17	11	119.778	0.035441	369.203	712.992	-0.000035765	0.00153114	2.11608
S 15	17	12	94.7471	0.232835	488.474	1193.04	-8.54586 ' 10 ⁻⁶	0.00108708	3.0283

Sample 15 Scan 18:

S	T	M	LL	w	s	t	a	% erg	f
S 15	18	1	1872.52	0.0215212	241.42	1133.21	0.0000545583	0.846265	-0.44803
S 15	18	2	778.167	0.0061368	552.277	1561.59	-4.5054815543121555 ' 10 ⁻⁶	0.0823077	0.559851
S 15	18	3	124.64	0.0277401	233.489	1520.83	0.000019003	0.00814	2.71007
S 15	18	4	304.224	0.0228976	375.16	728.545	4.8199858238328345 ' 10 ⁻⁶	0.0160851	-2.74329
S 15	18	5	302.047	0.0842052	335.795	848.946	-0.0000305745	0.0117932	0.186287
S 15	18	6	109.186	0.0593602	698.089	980.038	-3.4362864648379634 ' 10 ⁻⁶	0.00345932	-1.68589
S 15	18	7	118.136	0.0419807	199.456	723.242	-1.0047943373801873 ' 10 ⁻⁶	0.00334072	1.29898
S 15	18	8	96.0861	0.0732097	176.84	1193.28	2.18696 ' 10 ⁻⁶	0.00239366	1.42974
S 15	18	9	328.819	0.139632	99.7375	900.	-9.99908 ' 10 ⁻⁷	0.00508683	-0.138396
S 15	18	10	79.1923	0.00573747	500.383	359.237	-0.0000114553	0.00145907	3.0794
S 15	18	11	175.894	0.118576	271.965	940.056	0.0000108931	0.00282384	-0.512574
S 15	18	12	97.3527	0.232881	475.772	1209.16	-7.47105 ' 10 ⁻⁶	0.00136219	-0.891232

Sample 15 Scan 19:

S	T	M	LL	w	s	t	a	% erg	f
S 15	19	1	1882.88	0.0218605	241.299	1129.91	0.0000548202	0.847849	-0.397789
S 15	19	2	771.383	0.00615622	550.543	1562.45	-4.53999 ' 10 ⁻⁶	0.0809862	0.553931
S 15	19	3	252.604	0.0234077	805.214	939.608	-4.04887 ' 10 ⁻⁶	0.0154469	-0.864738
S 15	19	4	275.078	0.0834344	348.123	842.714	-0.0000297436	0.012925	0.7892
S 15	19	5	105.319	0.0595366	694.717	1005.56	-3.06976 ' 10 ⁻⁶	0.00408049	3.02253
S 15	19	6	168.992	0.0372217	157.059	639.666	-0.0000528638	0.00571242	-0.971127
S 15	19	7	122.976	0.0170087	413.761	1491.5	-2.5386 ' 10 ⁻⁶	0.00359007	2.70185
S 15	19	8	145.742	0.0340193	375.441	1219.87	-6.88796 ' 10 ⁻⁷	0.00372071	0.904184
S 15	19	9	145.759	0.0727166	173.132	1200.	-1.0000009788210643 ' 10 ⁻⁶	0.00272706	1.01993
S 15	19	10	375.924	0.139645	100.384	900.	-9.13321 ' 10 ⁻⁷	0.00431002	-0.0598138
S 15	19	11	159.537	0.119655	291.221	903.218	0.0000141753	0.00245925	-2.36213
S 15	19	12	174.415	0.00841692	161.174	209.716	-0.0000577048	0.00227562	-1.78783

Sample 15 Scan 20:

S	T	M	LL	w	s	t	a	% erg	f
S 15	20	1	1780.48	0.0227394	243.057	1118.66	0.0000550458	0.831443	-0.243293
S 15	20	2	598.088	0.00615213	543.074	1556.75	-4.63397 ' 10 ⁻⁶	0.0752392	0.573199
S 15	20	3	171.781	0.0233962	824.274	940.395	-4.21914 ' 10 ⁻⁶	0.0144365	-0.93025
S 15	20	4	434.472	0.088955	223.473	934.789	-0.0000302963	0.0219288	-0.927362
S 15	20	5	145.968	0.0585692	740.524	901.747	-3.13955 ' 10 ⁻⁶	0.0074824	2.52589
S 15	20	6	141.848	0.07207	772.534	1226.52	-1.1528154661430103 ' 10 ⁻⁶	0.00629631	-0.917797
S 15	20	7	169.017	0.0365521	363.249	598.047	-0.0000259467	0.00642453	0.243825
S 15	20	8	182.517	0.0340647	111.537	1213.4	0.000595987	0.00582055	0.149061
S 15	20	9	392.201	0.140963	97.0214	899.999	-1. ' 10 ⁻⁶	0.00647793	0.153659
S 15	20	10	193.86	0.117876	206.856	901.026	0.0000122469	0.00372845	-1.83762
S 15	20	11	131.697	0.145397	5634.84	15611.8	-5.88154 ' 10 ⁻⁶	0.00231222	2.83674
S 15	20	12	68.5929	0.0341323	1485.11	1593.86	2.64094 ' 10 ⁻⁷	0.00108892	0.487782

Sample 15 Scan 21:

S	T	M	LL	w	s	t	a	% erg	f
S 15	21	1	1450.76	0.0238849	244.367	1102.39	0.0000550544	0.765609	-0.0288668
S 15	21	2	323.466	0.00600688	534.677	1535.73	-4.68146' 10 ⁻⁶	0.0644315	0.66723
S 15	21	3	407.469	0.0888951	232.833	978.575	-0.0000191155	0.0422952	0.873986
S 15	21	4	110.369	0.071925	732.149	1137.69	-6.32995' 10 ⁻⁷	0.0131749	-1.35204
S 15	21	5	95.7715	0.0587389	740.308	929.4	-2.80847' 10 ⁻⁶	0.0103114	0.431219
S 15	21	6	72.7451	0.03041	302.432	1449.33	0.0000179246	0.00719817	-1.79031
S 15	21	7	156.937	0.0228976	410.934	726.908	5.9625' 10 ⁻⁶	0.0138554	-3.02124
S 15	21	8	324.109	0.139257	136.234	900.	-1.0003435969165067' 10 ⁻⁶	0.0209688	0.0564061
S 15	21	9	450.641	0.12346	175.552	986.823	-7.89337' 10 ⁻⁶	0.0134782	0.409211
S 15	21	10	92.904	0.232497	450.699	1204.26	-5.7025353052541265' 10 ⁻⁶	0.00417802	0.377602
S 15	21	11	91.1162	0.0991508	743.129	956.781	-1.8424' 10 ⁻⁶	0.00373737	2.18336
S 15	21	12	103.367	0.13161	85.0223	813.396	-3.6540696669827117' 10 ⁻⁶	0.0036557	1.80186

Sample 15 Scan 22:

S	T	M	LL	w	s	t	a	% erg	f
S 15	22	1	1555.7	0.0235444	245.51	1107.29	0.000054753	0.788959	-0.0844464
S 15	22	2	393.349	0.00604481	538.714	1544.47	-4.63294' 10 ⁻⁶	0.068186	0.635348
S 15	22	3	398.48	0.0905588	154.627	963.691	-0.0000331027	0.03577	2.47811
S 15	22	4	144.718	0.0719653	729.017	1099.47	-9.07941' 10 ⁻⁷	0.0141921	1.64383
S 15	22	5	88.6436	0.0303119	336.318	1447.18	0.0000184214	0.00773144	-1.66759
S 15	22	6	117.642	0.0586971	759.117	936.604	-3.08562' 10 ⁻⁶	0.00925735	0.161397
S 15	22	7	216.689	0.0229386	405.277	724.081	5.9150465669250555' 10 ⁻⁶	0.0144465	-2.90722
S 15	22	8	490.953	0.124727	155.885	1000.	-1.' 10 ⁻⁶	0.0171662	-0.825234
S 15	22	9	72.6543	0.232877	464.158	1237.59	-4.39157' 10 ⁻⁶	0.00298114	-1.13592
S 15	22	10	90.2869	0.0444258	214.389	800.	-1.0000654150856763' 10 ⁻⁶	0.00341246	-2.53596
S 15	22	11	164.115	0.144799	231.694	1000.	-1.0161417388256785' 10 ⁻⁶	0.00545358	-1.51412
S 15	22	12	101.129	0.0850918	172.848	1300.	-1.0000687246729552' 10 ⁻⁶	0.00198854	-2.34079

Sample 15 Scan 23:

S	T	M	LL	w	s	t	a	% erg	f
S 15	23	1	1441.54	0.0238364	245.585	1103.08	0.0000548649	0.763437	-0.0312969
S 15	23	2	320.44	0.00601217	538.245	1540.42	-4.6343946614950535' 10 ⁻⁶	0.0645046	0.650743
S 15	23	3	624.665	0.0897493	246.387	984.379	-0.0000208265	0.0427164	0.373398
S 15	23	4	102.336	0.0719041	788.429	1190.28	-7.2345' 10 ⁻⁷	0.0124215	1.19678
S 15	23	5	97.5247	0.0587248	746.382	925.361	-2.7371571329135256' 10 ⁻⁶	0.0107114	0.67615
S 15	23	6	73.0054	0.0302988	301.926	1451.45	0.0000191369	0.0073617	-1.85698
S 15	23	7	155.402	0.0229671	405.348	720.351	5.8959561424202345' 10 ⁻⁶	0.0139901	-2.86128
S 15	23	8	386.96	0.123813	250.022	1000.	-1.' 10 ⁻⁶	0.0199754	-0.895956
S 15	23	9	261.621	0.140857	236.856	900.	-1.' 10 ⁻⁶	0.0143779	0.330369
S 15	23	10	93.2594	0.232763	438.918	1234.73	-4.76006' 10 ⁻⁶	0.00435046	-0.254735
S 15	23	11	146.215	0.111426	231.86	1100.	-1.' 10 ⁻⁶	0.00385501	0.70097
S 15	23	12	106.434	0.0431602	196.711	710.202	-9.68735' 10 ⁻⁷	0.00410283	1.37535

Sample 15 Scan 24:

S	T	M	LL	w	s	t	a	% erg	f
S 15	24	1	1369.96	0.0239373	245.607	1100.79	0.0000548382	0.745884	-0.0102611
S 15	24	2	284.68	0.00597413	536.926	1535.24	-4.64628' 10 ⁻⁶	0.0626474	0.673453
S 15	24	3	465.748	0.0893389	243.701	978.969	-0.0000206206	0.0454704	0.728577
S 15	24	4	91.433	0.0719151	759.549	1183.1	-5.44979' 10 ⁻⁷	0.0126191	1.60048
S 15	24	5	86.5781	0.0587424	747.08	924.368	-2.63005' 10 ⁻⁶	0.0109311	0.628868
S 15	24	6	61.2088	0.03034	299.546	1448.36	0.0000189187	0.00717643	-1.80517
S 15	24	7	358.318	0.138836	135.661	900.	-9.39551' 10 ⁻⁷	0.0248921	-0.101069
S 15	24	8	169.387	0.0229399	402.424	718.259	5.7365695355950995' 10 ⁻⁶	0.0138368	-2.8398
S 15	24	9	328.52	0.118503	179.	1000.	-1.0389' 10 ⁻⁶	0.0183567	-1.18207
S 15	24	10	105.492	0.23297	438.772	1246.93	-5.70998' 10 ⁻⁶	0.00566746	3.13191
S 15	24	11	68.0268	0.127601	160.755	700.	-1.' 10 ⁻⁶	0.00232575	-2.33159
S 15	24	12	84.0985	0.0966862	207.162	617.955	-1.5533607744838807' 10 ⁻⁶	0.00392121	-2.29364

Sample 15 Scan 25:

S	T	M	LL	w	s	t	a	% erg	f
S 15	25	1	1372.62	0.0238696	245.58	1101.27	0.0000547701	0.746558	-0.0219432
S 15	25	2	291.19	0.0060082	537.173	1536.9	-4.6928851256837865 ' 10 ⁻⁶	0.0637067	0.664334
S 15	25	3	386.805	0.090019	207.896	990.291	-0.0000206879	0.0458046	-0.313239
S 15	25	4	109.069	0.0718776	747.788	1122.84	-3.2676216776753744 ' 10 ⁻⁷	0.014708	-0.390392
S 15	25	5	90.3149	0.0587098	742.6	925.104	-2.70087 ' 10 ⁻⁶	0.0110217	0.601154
S 15	25	6	63.8305	0.0301648	296.375	1451.4	0.0000190052	0.00721057	-1.89509
S 15	25	7	276.519	0.138699	121.275	900.	-9.61551 ' 10 ⁻⁷	0.0238653	-0.14501
S 15	25	8	230.138	0.118504	176.561	999.999	-1.0092606138046703 ' 10 ⁻⁶	0.0163399	-1.29098
S 15	25	9	226.298	0.0229557	403.599	718.937	5.8467703543549164 ' 10 ⁻⁶	0.0140128	-2.86024
S 15	25	10	154.073	0.217435	404.663	999.526	-0.0000363011	0.00787908	-2.83539
S 15	25	11	61.7661	0.127386	197.735	711.016	-1.00722 ' 10 ⁻⁶	0.00283213	2.34651
S 15	25	12	96.982	0.0434507	199.247	711.129	-9.6803 ' 10 ⁻⁷	0.00410937	1.27346

Sample 15 Scan 26:

S	T	M	LL	w	s	t	a	% erg	f
S 15	26	1	1243.67	0.024013	245.616	1097.69	0.0000548553	0.711675	0.00444241
S 15	26	2	234.005	0.00604747	534.965	1538.51	-4.68376 ' 10 ⁻⁶	0.0599113	0.637967
S 15	26	3	355.283	0.0912486	252.358	1009.36	-0.0000215584	0.0493577	-2.23553
S 15	26	4	77.5631	0.0718148	788.284	1171.69	-3.9217446264145745 ' 10 ⁻⁷	0.0132503	2.22492
S 15	26	5	69.8921	0.0587383	758.621	922.83	-2.4376859516132255 ' 10 ⁻⁶	0.0110907	0.556236
S 15	26	6	266.396	0.138937	206.638	900.108	-1. ' 10 ⁻⁶	0.0296108	-0.214208
S 15	26	7	203.581	0.120811	179.049	999.998	-8.98829 ' 10 ⁻⁷	0.0219839	-1.38089
S 15	26	8	68.2171	0.0302467	296.185	1449.8	0.0000193849	0.00670024	-1.91386
S 15	26	9	150.702	0.0229938	384.576	705.208	5.54939 ' 10 ⁻⁶	0.0132771	-2.58066
S 15	26	10	109.292	0.233729	431.766	1289.31	-6.37333 ' 10 ⁻⁶	0.00845126	-0.714654
S 15	26	11	212.397	0.20792	155.931	788.969	-0.0000145343	0.00863885	-2.78278
S 15	26	12	65.1817	0.0995592	710.5	900.928	-8.48354 ' 10 ⁻⁷	0.00407264	0.809748

Sample 15 Scan 27:

S	T	M	LL	w	s	t	a	% erg	f
S 15	27	1	1313.03	0.0237923	246.234	1100.12	0.0000548117	0.730997	-0.0349407
S 15	27	2	264.825	0.00604787	537.712	1540.87	-4.64551 ' 10 ⁻⁶	0.062301	0.628801
S 15	27	3	321.921	0.0912495	130.952	1010.3	-0.0000212173	0.0436812	-2.34203
S 15	27	4	142.671	0.0720455	605.788	1000.27	8.92523 ' 10 ⁻⁷	0.0214657	1.74216
S 15	27	5	85.6059	0.0585596	672.909	892.652	-3.30733 ' 10 ⁻⁶	0.0114844	2.47117
S 15	27	6	283.071	0.13879	145.741	900.276	-1. ' 10 ⁻⁶	0.0263738	-0.28075
S 15	27	7	174.425	0.122475	264.319	1000.01	-9.99914 ' 10 ⁻⁷	0.015286	-1.63019
S 15	27	8	83.9172	0.0299559	292.156	1456.82	0.0000199451	0.00698947	-2.12111
S 15	27	9	191.111	0.0230103	379.011	702.694	5.316 ' 10 ⁻⁶	0.0138895	-2.49728
S 15	27	10	118.127	0.23382	416.893	1303.86	-6.90411 ' 10 ⁻⁶	0.00734843	2.19287
S 15	27	11	44.6862	0.0720219	4938.9	8447.96	4.4596652174782484 ' 10 ⁻⁷	0.00256122	-1.33377
S 15	27	12	147.315	0.208943	212.1	830.98	-0.0000192656	0.00650946	1.13344

Sample 15 Scan 28:

S	T	M	LL	w	s	t	a	% erg	f
S 15	28	1	1158.33	0.0239919	246.962	1095.87	0.0000548554	0.68599	0.00315327
S 15	28	2	204.902	0.00605286	535.957	1538.39	-4.65302 ' 10 ⁻⁶	0.0579651	0.628628
S 15	28	3	448.119	0.0897842	235.333	948.352	-0.000025804	0.0550966	-3.07507
S 15	28	4	321.966	0.138647	184.182	900.	-9.31659 ' 10 ⁻⁷	0.0336833	-0.417473
S 15	28	5	159.229	0.120859	199.787	1000.	-1.0005353292880292 ' 10 ⁻⁶	0.0242547	-1.65023
S 15	28	6	77.8498	0.0720282	795.759	1303.35	-6.73306 ' 10 ⁻⁷	0.0106011	-0.966466
S 15	28	7	87.2456	0.058797	779.17	916.826	-2.20881 ' 10 ⁻⁶	0.0109399	0.75595
S 15	28	8	56.3833	0.0303105	294.684	1447.26	0.0000207629	0.00657887	-1.91473
S 15	28	9	133.386	0.234034	410.497	1311.91	-7.13794 ' 10 ⁻⁶	0.0141633	0.0849816
S 15	28	10	139.861	0.0231114	372.999	694.615	5.46239 ' 10 ⁻⁶	0.0129554	-2.37987
S 15	28	11	120.809	0.213086	487.688	1016.98	-4.68883 ' 10 ⁻⁶	0.00982104	-1.10002
S 15	28	12	73.2371	0.122747	1135.09	1436.18	-0.0000122525	0.00540116	-0.864567

Sample 15 Scan 29:

S	T	M	LL	w	s	t	a	% erg	f
S 15	29	1	1166.55	0.023751	246.998	1097.43	0.0000552473	0.68856	-0.0531369
S 15	29	2	211.609	0.00605562	536.943	1535.17	-4.70331 ' 10 ⁻⁶	0.0591836	0.632545
S 15	29	3	225.38	0.089641	189.985	1000.	-1.0044774077339316 ' 10 ⁻⁶	0.0490879	-1.74805
S 15	29	4	82.1699	0.0718681	721.388	1046.19	9.28931 ' 10 ⁻⁷	0.0159142	-1.76714
S 15	29	5	236.022	0.12479	196.808	999.446	-9.99257 ' 10 ⁻⁷	0.0387668	-1.48257
S 15	29	6	74.6553	0.0586887	761.762	904.17	-2.1231249572363873 ' 10 ⁻⁶	0.0105789	1.46274
S 15	29	7	52.0714	0.0303071	292.052	1448.72	0.0000215706	0.00692484	-1.99838
S 15	29	8	200.081	0.14152	153.498	900.001	-9.76042 ' 10 ⁻⁷	0.01906	-0.168764
S 15	29	9	128.246	0.233878	417.427	1299.05	-6.28963 ' 10 ⁻⁶	0.0132995	3.13772
S 15	29	10	147.632	0.0231902	360.735	687.548	5.29246 ' 10 ⁻⁶	0.0133402	-2.20594
S 15	29	11	267.887	0.20912	209.567	832.756	-0.0000121186	0.0118672	0.543621
S 15	29	12	93.1691	0.125937	663.317	1063.16	4.84413 ' 10 ⁻⁶	0.00640407	0.563364

Sample 15 Scan 30:

S	T	M	LL	w	s	t	a	% erg	f
S 15	30	1	1484.1	0.0229635	246.903	1109.07	0.0000550661	0.773293	-0.195134
S 15	30	2	371.259	0.00606387	544.273	1543.45	-4.6673 ' 10 ⁻⁶	0.0699015	0.61822
S 15	30	3	274.113	0.0878356	297.578	917.446	-0.0000267891	0.0371917	0.0142817
S 15	30	4	132.525	0.0233153	804.727	914.117	-3.98945 ' 10 ⁻⁶	0.0146377	-0.51683
S 15	30	5	95.4443	0.0587927	748.852	922.708	-2.7118954397889327 ' 10 ⁻⁶	0.00940245	0.790356
S 15	30	6	225.455	0.124292	254.607	999.962	-1.0032094931994964 ' 10 ⁻⁶	0.0167585	-1.20074
S 15	30	7	99.0791	0.0720492	581.319	1396.8	-4.19009 ' 10 ⁻⁷	0.00727535	-1.12372
S 15	30	8	222.719	0.140142	190.25	900.	-1.00003 ' 10 ⁻⁶	0.0107167	0.145592
S 15	30	9	123.323	0.0407442	387.142	662.96	-0.0000251971	0.00686097	-2.60098
S 15	30	10	83.0376	0.0319986	675.415	1167.33	-3.7713475688520774 ' 10 ⁻⁶	0.00416539	2.25835
S 15	30	11	83.4928	0.0858694	394.127	1235.32	-0.0000119512	0.00385361	-3.02628
S 15	30	12	103.688	0.234315	418.942	1316.19	-6.47572 ' 10 ⁻⁶	0.00435884	-0.619794

Sample 15 Scan 31:

S	T	M	LL	w	s	t	a	% erg	f
S 15	31	1	1482.6	0.0228062	245.928	1110.11	0.0000553478	0.772955	-0.233115
S 15	31	2	375.669	0.00605507	539.771	1538.08	-4.75368 ' 10 ⁻⁶	0.070699	0.640839
S 15	31	3	274.068	0.08767	298.595	909.924	-0.000027902	0.0370835	0.689693
S 15	31	4	137.854	0.023326	811.743	913.326	-4.0083661676831204 ' 10 ⁻⁶	0.0151454	-0.498679
S 15	31	5	89.8075	0.0629081	423.419	1498.16	-0.0000322542	0.00880054	-1.88752
S 15	31	6	375.513	0.124366	88.858	1000.	-1. ' 10 ⁻⁶	0.0265717	-1.229
S 15	31	7	176.666	0.0446057	127.522	643.676	-0.0000784173	0.0108641	-1.6212
S 15	31	8	128.27	0.0739129	239.131	1100.	-1. ' 10 ⁻⁶	0.00672417	1.5589
S 15	31	9	64.1119	0.0170971	431.049	1482.8	-1.0138391028926606 ' 10 ⁻⁶	0.00307385	2.6304
S 15	31	10	97.513	0.234376	439.348	1308.64	-4.63013 ' 10 ⁻⁶	0.00431328	1.05028
S 15	31	11	66.5247	0.0977548	159.913	595.89	4.99268 ' 10 ⁻⁶	0.00269631	-0.190883
S 15	31	12	72.7133	0.0331407	1567.08	1336.18	-3.34598 ' 10 ⁻⁶	0.00276428	3.04985

Sample 15 Scan 32:

S	T	M	LL	w	s	t	a	% erg	f
S 15	32	1	1149.73	0.0234951	246.973	1098.76	0.0000553471	0.683277	-0.101868
S 15	32	2	209.791	0.0059998	536.657	1527.62	-4.81428 ' 10 ⁻⁶	0.0597322	0.67339
S 15	32	3	368.287	0.124691	66.0736	1000.43	-9.94016 ' 10 ⁻⁷	0.0766996	-1.73487
S 15	32	4	168.26	0.0746337	570.016	686.108	-0.0000258749	0.0277058	-0.524096
S 15	32	5	87.9362	0.0234343	823.252	936.276	-4.37707 ' 10 ⁻⁶	0.0127277	-1.10595
S 15	32	6	102.434	0.234513	424.468	1316.41	-5.17688 ' 10 ⁻⁶	0.0134811	-1.06102
S 15	32	7	81.9296	0.0711768	1041.03	1362.42	-5.33866 ' 10 ⁻⁶	0.00983145	1.34584
S 15	32	8	192.748	0.208936	209.59	837.676	-0.0000137261	0.0117936	-0.482402
S 15	32	9	113.756	0.054329	1281.03	679.384	-6.2116 ' 10 ⁻⁶	0.0111133	1.82111
S 15	32	10	128.601	0.091406	506.246	963.179	0.0000148847	0.011131	1.10053
S 15	32	11	82.5668	0.0360366	414.282	591.234	-0.0000229484	0.00642788	-0.0525994
S 15	32	12	122.743	0.136397	177.188	700.219	-9.63674 ' 10 ⁻⁷	0.00485942	2.64757

Sample 15 Scan 33:

S	T	M	LL	w	s	t	a	% erg	f
S 15	33	1	1155.36	0.0233768	247.185	1099.43	0.0000553735	0.685056	-0.121887
S 15	33	2	212.598	0.00602958	537.073	1529.77	-4.7705072686118415 ' 10 ⁻⁶	0.0601126	0.65497
S 15	33	3	234.412	0.089523	195.801	999.926	-1. ' 10 ⁻⁶	0.0495964	-1.8346
S 15	33	4	215.557	0.124355	257.319	1000.	-9.99494 ' 10 ⁻⁷	0.0362097	-1.6352
S 15	33	5	94.9554	0.071812	747.762	1063.34	1.0435 ' 10 ⁻⁶	0.015188	-3.03547
S 15	33	6	166.282	0.139839	239.187	900.	-1.0217867446693128 ' 10 ⁻⁶	0.0227549	-0.232556
S 15	33	7	83.3049	0.0586791	781.322	898.199	-1.7902900062881998 ' 10 ⁻⁶	0.0103685	1.73128
S 15	33	8	111.22	0.0244099	815.469	1066.44	-4.3821836003208535 ' 10 ⁻⁶	0.0125627	2.05324
S 15	33	9	110.328	0.23422	418.627	1296.59	-3.26763 ' 10 ⁻⁶	0.0111549	-2.6364
S 15	33	10	222.226	0.209722	225.063	862.505	-0.0000115335	0.0116365	0.645944
S 15	33	11	88.1525	0.0349951	134.543	598.017	-0.0000478941	0.0070874	-0.105817
S 15	33	12	32.9696	0.0792617	2568.12	2596.26	-2.96301 ' 10 ⁻⁷	0.00249423	0.400342

Sample 15 Scan 34:

S	T	M	LL	w	s	t	a	% erg	f
S 15	34	1	1163.2	0.0233064	247.898	1099.38	0.000055442	0.687516	-0.134068
S 15	34	2	214.95	0.00605798	539.939	1532.99	-4.71979 ' 10 ⁻⁶	0.0602354	0.629812
S 15	34	3	242.407	0.0897258	169.94	1000.12	-1. ' 10 ⁻⁶	0.0494269	-1.88238
S 15	34	4	86.8172	0.0719902	684.346	1036.36	1.4135909285149022 ' 10 ⁻⁶	0.0167537	-1.18752
S 15	34	5	359.234	0.12342	104.774	1000.37	-9.75755 ' 10 ⁻⁷	0.0554941	-1.63839
S 15	34	6	85.0402	0.058755	789.76	903.424	-1.66791 ' 10 ⁻⁶	0.0105352	1.35748
S 15	34	7	117.627	0.0232794	785.875	898.857	-3.91355 ' 10 ⁻⁶	0.0131716	-0.321059
S 15	34	8	180.677	0.207098	234.133	879.613	-0.0000453452	0.0167792	-2.63514
S 15	34	9	99.6198	0.235405	116.515	1400.45	-1.0021602576455904 ' 10 ⁻⁶	0.00707792	-2.02034
S 15	34	10	149.614	0.140935	276.56	778.967	-0.0000412281	0.0113472	-1.49605
S 15	34	11	39.3379	0.078458	2830.24	3358.57	2.56681 ' 10 ⁻⁸	0.00271219	-2.45388
S 15	34	12	110.578	0.0387454	353.527	610.355	-0.0000268288	0.00707651	-0.742452

Sample 15 Scan 35:

S	T	M	LL	w	s	t	a	% erg	f
S 15	35	1	1158.22	0.023339	248.854	1099.32	0.0000550565	0.685955	-0.117073
S 15	35	2	212.969	0.00604596	541.483	1536.18	-4.64375 ' 10 ⁻⁶	0.0600272	0.622393
S 15	35	3	239.31	0.089645	160.896	1000.	-9.99519 ' 10 ⁻⁷	0.0497534	-1.85951
S 15	35	4	90.1614	0.0720386	655.07	1030.15	1.5292194247746144 ' 10 ⁻⁶	0.0174892	-0.771723
S 15	35	5	371.613	0.1248	99.6966	1000.31	0.0000232822	0.0565872	-1.70056
S 15	35	6	87.0168	0.0587348	771.825	895.72	-1.7100326348066428 ' 10 ⁻⁶	0.010732	1.81246
S 15	35	7	117.541	0.0232042	780.539	891.71	-3.9090450438734335 ' 10 ⁻⁶	0.0130907	-0.149338
S 15	35	8	237.418	0.210617	222.503	896.916	-0.00001152	0.0139793	-0.347192
S 15	35	9	100.594	0.235472	375.405	1303.27	-5.90034 ' 10 ⁻⁶	0.00870573	2.07967
S 15	35	10	115.385	0.139917	290.045	762.196	-0.0000449453	0.00896479	0.91259
S 15	35	11	99.6729	0.0391224	710.177	622.041	-0.0000294679	0.0069536	-1.0891
S 15	35	12	144.555	0.331604	47.4478	1099.91	-1.0008252877951381 ' 10 ⁻⁶	0.00847874	-1.33707

Sample 15 Scan 36:

S	T	M	LL	w	s	t	a	% erg	f
S 15	36	1	1155.39	0.0231864	249.527	1100.31	0.0000551636	0.685067	-0.14607
S 15	36	2	215.003	0.00607684	542.634	1537.83	-4.6559605021627125 ' 10 ⁻⁶	0.0607157	0.606667
S 15	36	3	254.204	0.0894271	186.511	1000.	-1.00001 ' 10 ⁻⁶	0.0517641	-1.88875
S 15	36	4	78.3753	0.0718762	711.853	1050.99	1.3350505353707346 ' 10 ⁻⁶	0.0151564	-2.23472
S 15	36	5	371.655	0.123162	95.7148	1001.33	-1. ' 10 ⁻⁶	0.0558405	-1.75487
S 15	36	6	86.0197	0.0587446	788.665	900.518	-1.5406324413375074 ' 10 ⁻⁶	0.0107202	1.50104
S 15	36	7	105.989	0.0284291	1542.66	1403.36	-5.30954 ' 10 ⁻⁶	0.0120016	-0.508464
S 15	36	8	125.307	0.212527	420.748	1007.02	-5.99082 ' 10 ⁻⁶	0.0126419	1.37024
S 15	36	9	88.1684	0.0340927	107.068	593.469	-0.0000489816	0.00799188	0.0251134
S 15	36	10	107.61	0.236034	284.794	1311.55	-9.32997 ' 10 ⁻⁶	0.00884577	0.191235
S 15	36	11	158.862	0.14225	294.815	792.344	-0.0000409292	0.0114364	2.86958
S 15	36	12	38.0588	0.0866762	5263.53	8373.96	-5.57992 ' 10 ⁻⁷	0.00248045	1.27401

Sample 15 Scan 37:

S	T	M	LL	w	s	t	a	% erg	f
S 15	37	1	1153.1	0.0231082	250.067	1100.96	0.0000549779	0.684344	-0.154391
S 15	37	2	216.169	0.0060861	543.981	1539.91	-4.65352 ' 10 ⁻⁶	0.0611477	0.599211
S 15	37	3	259.582	0.0893136	195.488	1000.	-9.99722 ' 10 ⁻⁷	0.0524707	-1.89758
S 15	37	4	73.8035	0.071815	724.344	1055.75	1.29836 ' 10 ⁻⁶	0.0142732	-2.58358
S 15	37	5	358.112	0.12334	95.037	1000.82	-1. ' 10 ⁻⁶	0.0551667	-1.70084
S 15	37	6	85.6902	0.0587302	788.873	900.415	-1.55624 ' 10 ⁻⁶	0.0107726	1.50487
S 15	37	7	105.202	0.0284432	1509.73	1400.34	-5.37995 ' 10 ⁻⁶	0.0120234	-0.414003
S 15	37	8	243.397	0.209641	202.439	881.16	-0.0000133545	0.0136172	3.06187
S 15	37	9	87.2859	0.0340002	109.587	592.907	-0.000049967	0.00792095	0.0429253
S 15	37	10	102.936	0.237336	252.148	1354.7	-6.58388 ' 10 ⁻⁶	0.00849462	2.5518
S 15	37	11	61.1608	0.127436	1683.07	1615.32	-0.0000128378	0.00464829	2.0938
S 15	37	12	49.1515	0.0179587	1496.13	1546.76	-0.0000129096	0.0035349	2.05369

Sample 15 Scan 38:

S	T	M	LL	w	s	t	a	% erg	f
S 15	38	1	1160.91	0.0230193	250.782	1101.57	0.0000550712	0.6868	-0.170611
S 15	38	2	221.127	0.00609733	544.391	1539.84	-4.68861 ' 10 ⁻⁶	0.0619167	0.597999
S 15	38	3	265.915	0.0892983	203.222	1000.	-1.0001544443573796 ' 10 ⁻⁶	0.0531324	-1.89174
S 15	38	4	72.953	0.071766	741.243	1064.51	1.1884448093533903 ' 10 ⁻⁶	0.0138424	3.10028
S 15	38	5	360.662	0.123066	95.939	999.755	-1. ' 10 ⁻⁶	0.0553132	-1.53565
S 15	38	6	88.9574	0.0587312	794.114	899.477	-1.4557274113820272 ' 10 ⁻⁶	0.0108602	1.55548
S 15	38	7	110.6	0.0283359	1508.82	1395.16	-5.30535 ' 10 ⁻⁶	0.0122224	-0.269659
S 15	38	8	131.803	0.212479	443.15	1028.31	-5.81457 ' 10 ⁻⁶	0.0129056	-3.07416
S 15	38	9	92.9055	0.0341352	106.879	593.56	-0.0000512317	0.00812721	0.0313512
S 15	38	10	111.785	0.236542	267.123	1309.42	-0.0000137025	0.00882871	0.889877
S 15	38	11	150.765	0.140627	291.851	768.896	-0.0000440703	0.0104469	-0.0302609
S 15	38	12	58.0778	0.0179603	1443.79	1545.02	-0.0000129913	0.0036224	2.09402

Sample 15 Scan 39:

S	T	M	LL	w	s	t	a	% erg	f
S 15	39	1	1295.01	0.0227607	251.179	1105.7	0.0000549395	0.726105	-0.214542
S 15	39	2	279.573	0.00610588	546.588	1543.68	-4.68721 ' 10 ⁻⁶	0.0665106	0.590884
S 15	39	3	285.329	0.0890612	197.538	1000.12	-1.0002883833439113 ' 10 ⁻⁶	0.0495182	-1.7512
S 15	39	4	91.1013	0.0717739	734.499	1067.21	1.2287833201922289 ' 10 ⁻⁶	0.013613	3.02716
S 15	39	5	96.4657	0.0281887	1494.91	1394.34	-5.13289 ' 10 ⁻⁶	0.0131247	-0.199551
S 15	39	6	437.686	0.122498	103.063	1000.	-9.37278 ' 10 ⁻⁷	0.0441941	-1.37069
S 15	39	7	133.918	0.0585969	759.515	871.928	-1.7782663022174238 ' 10 ⁻⁶	0.0107043	-2.9682
S 15	39	8	117.967	0.0337112	107.205	594.707	-0.0000505989	0.00831211	0.0531399
S 15	39	9	130.376	0.212552	433.833	1035.3	-5.73972 ' 10 ⁻⁶	0.00811453	1.90128
S 15	39	10	70.9779	0.0176589	1403.23	1537.48	-0.0000130104	0.00399255	2.29664
S 15	39	11	168.205	0.139691	295.02	759.188	-0.0000475437	0.0083879	1.60311
S 15	39	12	46.2157	0.0802062	2265.2	2517.82	-6.14408 ' 10 ⁻⁷	0.00206809	-0.231004

Sample 15 Scan 40:

S	T	M	LL	w	s	t	a	% erg	f
S 15	40	1	1543.48	0.0218286	249.928	1117.68	0.000054783	0.786364	-0.379056
S 15	40	2	445.956	0.00610146	550.838	1547.35	-4.68591 ' 10 ⁻⁶	0.0763877	0.594296
S 15	40	3	133.728	0.0234266	788.438	918.11	-3.85282 ' 10 ⁻⁶	0.0169673	-0.6282
S 15	40	4	285.155	0.0885666	255.747	1000.	-1. ' 10 ⁻⁶	0.0280627	-1.50071
S 15	40	5	101.425	0.0715205	832.944	1098.07	5.82499 ' 10 ⁻⁷	0.00873022	1.1967
S 15	40	6	112.163	0.0587505	821.027	900.867	-1.4612656688385938 ' 10 ⁻⁶	0.00867747	1.83783
S 15	40	7	424.457	0.121119	88.5569	1000.	-1.0692734299842495 ' 10 ⁻⁶	0.022623	-1.22056
S 15	40	8	173.454	0.0389506	373.433	619.995	-0.000026252	0.00803931	-0.900285
S 15	40	9	93.872	0.0328436	673.012	1278.72	-3.4934496041316275 ' 10 ⁻⁶	0.00380307	-1.40551
S 15	40	10	93.0342	0.0180972	1259.18	1658.2	-4.73863 ' 10 ⁻⁷	0.0034328	-0.434819
S 15	40	11	127.196	0.211871	389.789	1002.62	-6.9318054202749325 ' 10 ⁻⁶	0.00420508	2.59801
S 15	40	12	53.1877	0.0991259	238.22	1354.03	-0.0000131856	0.00160584	0.805085

Sample 15 Scan 41:

S	T	M	LL	W	S	t	a	% erg	f
S 15	41	1	1535.09	0.0218692	250.592	1116.93	0.0000549792	0.784564	-0.375226
S 15	41	2	441.587	0.00611178	547.772	1544.56	-4.77389 ' 10 ⁻⁶	0.076445	0.605975
S 15	41	3	133.379	0.0234723	797.471	921.466	-3.8750273728399305 ' 10 ⁻⁶	0.0171479	-0.706468
S 15	41	4	314.262	0.0885413	193.248	1000.	-1.0146970080868854 ' 10 ⁻⁶	0.032051	-1.46508
S 15	41	5	130.779	0.0717487	725.732	1070.24	1.3968614421095063 ' 10 ⁻⁶	0.010803	3.06321
S 15	41	6	184.285	0.0559427	-84.6369	602.096	0.000414561	0.0130132	-0.376474
S 15	41	7	90.7772	0.0589162	1098.33	1284.51	7.66796 ' 10 ⁻⁶	0.00558011	-2.71361
S 15	41	8	535.692	0.118373	93.1474	999.989	-9.46429 ' 10 ⁻⁷	0.0206948	-1.09376
S 15	41	9	108.753	0.0355397	756.6	1185.09	2.57294 ' 10 ⁻⁶	0.00391867	1.58534
S 15	41	10	138.808	0.210126	236.789	906.222	-0.0000108207	0.00382294	-1.98283
S 15	41	11	68.4399	0.0270779	485.626	423.614	-5.19018 ' 10 ⁻⁶	0.00200343	-0.908131
S 15	41	12	132.532	0.0187136	658.358	1646.86	-5.47371 ' 10 ⁻⁶	0.00351057	-0.0101471

Sample 15 Scan 42:

S	T	M	LL	W	S	t	a	% erg	f
S 15	42	1	1565.36	0.0217434	251.008	1118.97	0.0000547308	0.790987	-0.390447
S 15	42	2	466.417	0.00610158	549.631	1546.99	-4.73535 ' 10 ⁻⁶	0.077413	0.602938
S 15	42	3	144.07	0.0234849	796.765	924.317	-3.87719 ' 10 ⁻⁶	0.0174265	-0.745866
S 15	42	4	339.213	0.0884209	212.707	1000.	-9.37278 ' 10 ⁻⁷	0.0314538	-1.40035
S 15	42	5	124.049	0.0716288	751.94	1084.54	1.2747326976505238 ' 10 ⁻⁶	0.009449	2.1047
S 15	42	6	200.956	0.0559845	-85.423	602.456	0.000411541	0.0130248	-0.351158
S 15	42	7	98.7213	0.0584486	1074.81	1308.36	7.72065 ' 10 ⁻⁶	0.00550062	2.20302
S 15	42	8	388.602	0.118412	248.687	1000.	-9.97082 ' 10 ⁻⁷	0.0127513	-0.948771
S 15	42	9	280.397	0.139257	228.779	900.	-1.00582 ' 10 ⁻⁶	0.00518771	0.131206
S 15	42	10	118.981	0.0354231	743.425	1203.44	2.4345291153236805 ' 10 ⁻⁶	0.0039345	0.98551
S 15	42	11	65.4118	0.0270292	470.35	421.619	-5.4982661405546625 ' 10 ⁻⁶	0.00197173	-0.825873
S 15	42	12	134.827	0.018334	616.159	1609.75	-8.74756 ' 10 ⁻⁶	0.00367908	0.88227

Sample 15 Scan 43:

S	T	M	LL	W	S	t	a	% erg	f
S 15	43	1	1566.43	0.0214789	251.753	1121.	0.0000547331	0.791211	-0.434551
S 15	43	2	477.271	0.00612856	550.337	1549.14	-4.73472 ' 10 ⁻⁶	0.0787355	0.588161
S 15	43	3	149.748	0.0235515	807.687	934.223	-3.92764 ' 10 ⁻⁶	0.0178478	-0.970845
S 15	43	4	326.836	0.0885311	209.062	1000.	-1. ' 10 ⁻⁶	0.0305339	-1.44123
S 15	43	5	118.037	0.0716284	748.504	1081.7	1.3428769133572002 ' 10 ⁻⁶	0.00890061	2.27953
S 15	43	6	196.645	0.055987	-85.6874	602.049	0.000406245	0.0126824	-0.337481
S 15	43	7	95.2115	0.0583342	1085.98	1312.9	7.75478 ' 10 ⁻⁶	0.00529979	1.93808
S 15	43	8	512.464	0.118332	101.366	1000.	-9.37278 ' 10 ⁻⁷	0.0174427	-1.08229
S 15	43	9	111.097	0.0356572	737.609	1156.95	2.53807 ' 10 ⁻⁶	0.00374462	2.6278
S 15	43	10	126.872	0.0172415	445.6	1542.97	-6.66661 ' 10 ⁻⁶	0.00379719	1.97515
S 15	43	11	223.391	0.207865	84.675	897.947	-0.000013892	0.00434221	-0.0878981
S 15	43	12	88.608	0.0270608	459.169	426.456	-5.87138 ' 10 ⁻⁶	0.00201204	-0.942702

Sample 15 Scan 44:

S	T	M	LL	W	S	t	a	% erg	f
S 15	44	1	1483.98	0.0215713	252.917	1118.15	0.0000546687	0.773266	-0.414363
S 15	44	2	416.25	0.0061255	549.544	1547.23	-4.73355 ' 10 ⁻⁶	0.0767582	0.589249
S 15	44	3	124.984	0.0236131	812.794	939.113	-3.94156 ' 10 ⁻⁶	0.0174241	-1.12649
S 15	44	4	333.138	0.0884013	203.561	1001.1	-9.98683 ' 10 ⁻⁷	0.0366617	-1.67784
S 15	44	5	107.302	0.0716659	724.834	1078.84	1.6638688766666844 ' 10 ⁻⁶	0.00958562	2.29488
S 15	44	6	183.953	0.0316647	88.9677	626.955	0.000409998	0.0142192	-1.47498
S 15	44	7	448.813	0.1194	98.2065	1000.	-1.03871 ' 10 ⁻⁶	0.0228113	-1.22384
S 15	44	8	118.977	0.0579092	1125.6	1350.9	7.80988 ' 10 ⁻⁶	0.00533534	-0.350422
S 15	44	9	233.722	0.209821	186.757	864.415	-0.0000108055	0.00528877	0.45618
S 15	44	10	124.89	0.0334563	1813.53	1356.11	-3.5239354951876224 ' 10 ⁻⁶	0.00433696	2.38329
S 15	44	11	115.94	0.0168066	394.091	1501.93	-7.73927 ' 10 ⁻⁶	0.003569	2.66626
S 15	44	12	49.3241	0.0385251	1297.84	1136.02	-1.6917662679016509 ' 10 ⁻⁶	0.00139727	-2.9795

Sample 15 Scan 45:

S	T	M	LL	w	s	t	a	% erg	f
S 15	45	1	1435.44	0.0215073	253.918	1117.27	0.0000547958	0.761989	-0.425479
S 15	45	2	387.564	0.0061617	551.765	1548.55	-4.74471' 10^{-6}	0.0760711	0.569432
S 15	45	3	116.936	0.0236237	822.344	936.356	-3.9103783230097994' 10^{-6}	0.0176951	-1.09117
S 15	45	4	334.504	0.0885075	200.243	1000.2	-1.' 10^{-6}	0.0400998	-1.67763
S 15	45	5	100.688	0.071648	719.29	1084.12	1.8134899184879415' 10^{-6}	0.00982175	1.82591
S 15	45	6	227.766	0.0569013	147.641	600.	-9.76042' 10^{-7}	0.00974762	0.227433
S 15	45	7	242.737	0.12149	255.227	1000.	-1.0387642505881289' 10^{-6}	0.0165143	-1.32782
S 15	45	8	96.4718	0.139211	323.745	899.919	4.26524' 10^{-6}	0.00611157	-0.245914
S 15	45	9	69.0983	0.0336863	911.134	1135.65	-0.0000134907	0.00402889	-2.47655
S 15	45	10	88.3392	0.0124326	4042.15	2482.92	2.61802' 10^{-6}	0.00476135	-0.0672575
S 15	45	11	211.831	0.210513	223.115	900.053	-0.0000107099	0.00652291	-0.776545
S 15	45	12	105.626	0.0589429	336.563	1319.	2.3945014794242255' 10^{-6}	0.00451374	1.75692

Sample 15 Scan 46:

S	T	M	LL	w	s	t	a	% erg	f
S 15	46	1	1467.66	0.0211967	254.006	1120.91	0.0000546492	0.769535	-0.475541
S 15	46	2	418.205	0.00615535	551.784	1549.15	-4.7606390988748164' 10^{-6}	0.0783291	0.576675
S 15	46	3	128.02	0.0236953	820.265	946.051	-3.90944' 10^{-6}	0.0180833	-1.29019
S 15	46	4	336.591	0.0883064	202.922	1000.54	-9.90677' 10^{-7}	0.0376142	-1.64839
S 15	46	5	73.3236	0.0654573	259.598	1509.57	-0.0000261106	0.0067012	-2.78454
S 15	46	6	307.457	0.12128	112.401	999.989	-9.99908' 10^{-7}	0.0212152	-1.25002
S 15	46	7	105.812	0.0726039	451.812	830.026	-1.6768178350429833' 10^{-6}	0.00671386	1.56283
S 15	46	8	208.452	0.0473767	68.0568	613.472	0.000073332	0.0113184	-0.666202
S 15	46	9	86.7296	0.0357645	882.543	1106.91	2.3384218110662045' 10^{-6}	0.00405685	-2.02321
S 15	46	10	185.737	0.209477	231.01	886.295	-0.0000153005	0.00587995	2.14044
S 15	46	11	248.806	0.192333	233.267	914.107	-8.70463' 10^{-6}	0.00457371	3.0541
S 15	46	12	121.562	0.0177634	476.313	1564.01	-8.03897' 10^{-6}	0.00392869	1.64488

Sample 15 Scan 47:

S	T	M	LL	w	s	t	a	% erg	f
S 15	47	1	1505.1	0.0209658	254.888	1123.99	0.000054552	0.778004	-0.513053
S 15	47	2	457.201	0.00620696	550.847	1553.7	-4.79862' 10^{-6}	0.0809705	0.556026
S 15	47	3	143.575	0.0237268	839.042	958.5	-4.13875' 10^{-6}	0.0186296	-1.51926
S 15	47	4	352.563	0.0882115	205.928	1000.	-1.' 10^{-6}	0.0356988	-1.50509
S 15	47	5	70.6373	0.0607242	403.582	1518.97	0.0000229387	0.00579399	2.56621
S 15	47	6	117.314	0.0589611	523.784	775.616	-0.0000105948	0.0087627	-3.04479
S 15	47	7	205.52	0.121248	258.015	1000.	-9.99986' 10^{-7}	0.0122218	-1.13087
S 15	47	8	132.724	0.0355636	345.108	567.305	-0.0000230223	0.00723101	0.956059
S 15	47	9	117.874	0.0701534	318.369	636.985	-0.0000130229	0.00566472	-2.94477
S 15	47	10	85.2423	0.0183246	987.944	1671.79	-6.45416' 10^{-7}	0.00369991	-0.614166
S 15	47	11	111.377	0.106786	270.373	1000.	7.19582' 10^{-6}	0.00432607	-1.03274
S 15	47	12	105.696	0.139331	317.997	899.953	5.74235' 10^{-6}	0.00373657	-0.180746

Sample 15 Scan 48:

S	T	M	LL	w	s	t	a	% erg	f
S 15	48	1	1240.4	0.0216674	257.554	1112.42	0.0000548146	0.710731	-0.389889
S 15	48	2	280.461	0.00618345	550.527	1546.66	-4.79938' 10^{-6}	0.0704704	0.566909
S 15	48	3	348.167	0.0884296	198.398	999.996	-1.' 10^{-6}	0.0595108	-1.84608
S 15	48	4	102.712	0.0269728	1039.78	1292.54	-4.91142' 10^{-6}	0.0154081	2.58526
S 15	48	5	299.446	0.121704	110.212	1000.	-9.99722' 10^{-7}	0.0362891	-1.44508
S 15	48	6	112.521	0.0715439	711.674	1103.26	2.3415347045509213' 10^{-6}	0.0112967	0.17683
S 15	48	7	127.414	0.0561879	152.959	593.186	0.0000212116	0.0113412	0.292251
S 15	48	8	75.2693	0.0276729	600.835	723.439	-5.00106' 10^{-6}	0.0060552	3.11539
S 15	48	9	447.811	0.195188	-114.729	900.004	-1.0008251420417373' 10^{-6}	0.0199461	-0.638078
S 15	48	10	129.5	0.236334	160.339	1373.73	-3.7507551067025864' 10^{-6}	0.00617145	-1.94453
S 15	48	11	143.82	0.129203	119.696	600.	-1.' 10^{-6}	0.00476479	-2.43406
S 15	48	12	129.027	0.057766	725.506	1370.3	6.85134' 10^{-6}	0.00563779	-1.68217

Sample 15 Scan 49:

S	T	M	LL	w	s	t	a	% erg	f
S 15	49	1	1529.56	0.0207556	255.849	1126.05	0.0000543233	0.78337	-0.541363
S 15	49	2	484.735	0.00618993	554.376	1554.58	-4.76973 ' 10 ⁻⁶	0.0826928	0.55801
S 15	49	3	157.206	0.0237588	829.546	956.527	-3.95345 ' 10 ⁻⁶	0.0192284	-1.48522
S 15	49	4	365.51	0.0879252	206.488	1000.	-9.9875 ' 10 ⁻⁷	0.0342834	-1.47784
S 15	49	5	116.553	0.0588237	772.548	858.668	-7.33128 ' 10 ⁻⁷	0.00865384	-2.1268
S 15	49	6	118.192	0.0714997	705.98	1103.57	2.02121 ' 10 ⁻⁶	0.00780379	0.534637
S 15	49	7	208.242	0.121464	254.792	1000.	-1.0148005173694972 ' 10 ⁻⁶	0.0105768	-1.14305
S 15	49	8	177.101	0.0389107	369.277	620.239	-0.0000259776	0.00837896	-0.917366
S 15	49	9	98.8816	0.0192831	1652.38	2218.74	-7.63476 ' 10 ⁻⁷	0.00407158	1.6605
S 15	49	10	94.6064	0.032342	546.951	1197.6	-3.6103287403831063 ' 10 ⁻⁶	0.00353588	1.28759
S 15	49	11	114.723	0.107402	265.332	999.987	-9.37281 ' 10 ⁻⁷	0.00384087	-0.827584
S 15	49	12	367.969	0.194772	72.6756	899.975	-1.0387642505881289 ' 10 ⁻⁶	0.00727743	-0.56194

Sample 15 Scan 50:

S	T	M	LL	w	s	t	a	% erg	f
S 15	50	1	1592.69	0.0203281	255.224	1131.38	0.0000541183	0.796623	-0.610556
S 15	50	2	561.841	0.00620061	556.664	1557.68	-4.76043 ' 10 ⁻⁶	0.0868007	0.550285
S 15	50	3	190.981	0.023745	823.33	956.422	-3.89351 ' 10 ⁻⁶	0.0199445	-1.45293
S 15	50	4	358.079	0.0879229	224.057	999.806	-9.32687 ' 10 ⁻⁷	0.027661	-1.39276
S 15	50	5	121.155	0.0588001	779.859	854.715	-7.88399 ' 10 ⁻⁷	0.00765714	-1.79925
S 15	50	6	105.918	0.0712959	752.007	1123.49	1.8474513392943171 ' 10 ⁻⁶	0.0059748	-0.771908
S 15	50	7	162.177	0.0385914	369.02	616.027	-0.0000255421	0.00800571	-0.698433
S 15	50	8	240.826	0.12174	249.933	1000.	-1. ' 10 ⁻⁶	0.00820914	-1.12523
S 15	50	9	122.97	0.0195869	1731.59	2371.61	-7.822 ' 10 ⁻⁷	0.00431135	-1.29539
S 15	50	10	114.322	0.0323314	602.702	1213.28	-3.6232857813104305 ' 10 ⁻⁶	0.00355905	0.832936
S 15	50	11	151.366	0.106845	196.354	1000.	-1. ' 10 ⁻⁶	0.00327965	-0.852475
S 15	50	12	410.113	0.194454	103.866	900.002	-1. ' 10 ⁻⁶	0.0056816	-0.543118

Sample 15 Scan 51:

S	T	M	LL	w	s	t	a	% erg	f
S 15	51	1	1375.9	0.0209988	258.723	1120.46	0.0000544513	0.747388	-0.496988
S 15	51	2	371.522	0.00624268	554.094	1555.41	-4.80885 ' 10 ⁻⁶	0.0780013	0.533646
S 15	51	3	350.805	0.0879385	200.912	1000.	-9.99868 ' 10 ⁻⁷	0.0508697	-1.64969
S 15	51	4	162.167	0.0238253	839.324	961.051	-3.94057 ' 10 ⁻⁶	0.018282	-1.66844
S 15	51	5	100.316	0.0589567	835.259	856.425	-3.6369135573276787 ' 10 ⁻⁷	0.00991082	-2.25383
S 15	51	6	103.974	0.0714515	703.926	1116.05	2.26447 ' 10 ⁻⁶	0.009275	-0.596541
S 15	51	7	263.167	0.121926	254.723	1000.	-1.0008360002881072 ' 10 ⁻⁶	0.0182986	-1.26132
S 15	51	8	97.2647	0.107716	263.288	1000.	-9.37451 ' 10 ⁻⁷	0.00609232	-0.947037
S 15	51	9	146.654	0.0388394	366.019	613.894	-0.0000259335	0.00821953	-0.816045
S 15	51	10	361.641	0.194502	89.1085	899.826	-9.76042 ' 10 ⁻⁷	0.0111515	-0.441494
S 15	51	11	98.9795	0.0195123	1606.63	2151.19	-9.02219 ' 10 ⁻⁷	0.00385305	2.74685
S 15	51	12	99.5964	0.0323405	596.393	1207.45	-3.6211473302594537 ' 10 ⁻⁶	0.0035101	0.855336

Sample 15 Scan 52:

S	T	M	LL	w	s	t	a	% erg	f
S 15	52	1	1599.45	0.0201486	256.678	1133.08	0.0000541118	0.797993	-0.636206
S 15	52	2	579.496	0.00626125	556.38	1562.48	-4.80666 ' 10 ⁻⁶	0.0882255	0.524488
S 15	52	3	198.678	0.0238418	835.18	969.642	-3.91846 ' 10 ⁻⁶	0.0201685	-1.74685
S 15	52	4	404.595	0.0875411	216.08	1000.	-9.97734 ' 10 ⁻⁷	0.0286584	-1.30912
S 15	52	5	136.827	0.0588907	768.004	854.612	-3.8085118239468053 ' 10 ⁻⁷	0.00806863	-1.84235
S 15	52	6	117.463	0.0712047	730.226	1139.36	2.2289609606015463 ' 10 ⁻⁶	0.00609844	-1.92361
S 15	52	7	187.931	0.0386007	366.636	616.095	-0.000025701	0.00838284	-0.700426
S 15	52	8	116.477	0.0201029	1878.86	2619.63	-8.28061 ' 10 ⁻⁷	0.00445795	0.014603
S 15	52	9	229.548	0.121776	259.411	1000.01	-1. ' 10 ⁻⁶	0.00728161	-0.997919
S 15	52	10	134.145	0.0322741	602.637	1211.73	-3.6235948048502768 ' 10 ⁻⁶	0.00361569	0.905958
S 15	52	11	174.531	0.107033	240.82	1000.	-1.01481 ' 10 ⁻⁶	0.00312501	-0.6958
S 15	52	12	0	0	0	0	0	0	0

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