

AMS analysis 1.35 with beta JMS

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Hi everyone. JMS analysis software appears to be up and running. Please be aware that there will obviously be bugs in the code I haven't spotted. Please inform me ASAP, as I will put things right as soon as I can.

Improvements to v1.33

I'm not going to re-write the whole notes again, as most of the info has not changed since last time. One big thing is that the JMS time series plotter was really bad before, and now it should work in all conditions with all options set in anyway. Next the ratio finding routine to scale up the JMS data (mentioned below for a previous version) has been tweaked, and now will do the same as before, but only looks at points where the JMS signal is really significant (i.e. $3 \times \text{noise}$). This greatly improves the result and gets better numbers at low signal.

Also, you can now recalculate the SO₄ wave from the MS data using the JMS data alone. This is done by scaling up the JMS data into the MS matrix for the scanned m/z, and then using this data and the relationships in alices diagnostic plots an improved signal at other key SO₄ m/z's is generated.

The relationships used are

$$48/64=1$$

$$48/80=0.5$$

$$48/81=0.25$$

$$48/98=0.125$$

To use the improved data, hit the "Improve" button in the SO₄ section of the JMS tab. To look at the diagnostics, click "Diagnose", on the same tab. Also, if you change your mind you can revert to the data in the MS used before the SO₄ optimization by clicking on "Revert". This is done by replacing the raw ms counts in the destination masses, with the fragmentation scaling factor (mentioned above), multiplied by the JMS scaled m.z 48 counts. This is because the m/z 48 has very little SO₄ contribution. However, this method may result in a slight error as an organic contribution will be deducted from this improved so₄ signal. However, the organic interference in the SO₄ fragments is nearly an order of magnitude less than the so₄ contribution, meaning the effect is nearly negligible. However, always check if you have any strong organics in m/z 64,80,81,98 before you use this tool.

Notes for v1.33

After talking to Hugh we decided it would be best to use the JMS data as a source of high signal to noise data that is fed into the Mass Spectra Data. However, some of you who have used the JMS software before may have noticed that the JMS Airbeam is usually lower than the MS Airbeam etc. So to compensate for this, the JMS data has a scale factor applied to it, which is calculated by performing a least distance fit to JMS VS. MS scatter plot data. This number is calculated for each JMS mass. However, on

rare occasions this scale factor changes due to various hardware changes (such as retuning etc). If you want you can make this ratio semi-time dependant, you can define a time when the instrument performance changed, and then you will generate a new ratio in each period. This is discussed later.

The JMS data is loaded into the `jmsdata` folder. The JMS data is stored with 1 m/z per wave. e.g. one wave for mass 11, one for mass 28, one for mass 40 etc. Stick data and spectra data are in separate waves. Stick waves have 4 columns (diff, avg, open, closed) whereas the raw spectra have $20 \times 4 = 80$ columns (the 20 is the number of points per m/z scan). Due to the way the JMS mode works, stick recalculation is not appropriate. Also the non-stick data is only collected for $2/60^{\text{th}}$ of a JMS m/z scan time in order to determine the peak position of that m/z (at which position the stick measurements are made for the remaining scan time) and so the non-stick data are not subsequently used.

Errors are calculated for the JMS sticks using a similar but slightly modified version of James' `err_calc()` function, `jms_err_calc()`. Due to the logging software reporting MS sample times in JMS save data files, instead of JMS sample times (a bug which has been reported and will soon be fixed), the times used by the JMS error calculation are predicted using the scan times used in MS mode which are then scaled using the relative scan times used in the parameter menu for General Alternation mode of operation.

To use the software, simply start the panel in the usual way, type “`runme()`” in the command line in the usual way. This recompiles James' panel with the JMS additions. To load the data click appropriate tabs as per MS and TOF mode. Then calculate corrections and errors as usual. Then before progressing any further, its time to improve the MS data using the JMS data. Go to the JMS panel, and click “Get m/z list” to return a string showing all the m/z's scanned in JMS mode. The next 2 boxes allow any combination of these JMS m/z's to be imported/removed to the MS waves. When data is imported, all MS waves are automatically backed up (usually with a wave in `root:msdata:mssdiff_m/z`) with a different wave for each JMS m/z. The MS error waves are also backed up as JMS errors are also imported. The JMS data is scaled by the ratio talked about previously, as are the errors. The automatic ratio routine only has problems in the case of a purely noisy m/z channel. In this case, all the MS data is noise so JMS is potentially the only real source of signal, and is therefore imported with a scale factor of 1. It helps to do James' error calculation before importing JMS data in the MS waves, as this provides an estimate of the relative JMS and MS noise levels which are then used in the scale factor optimisation routine. Although recommended, it is not vital to calculate these errors on the corrections tab as the software provides a guess of the relative noise between MS and JMS mode.

The “plot diagnostics” button plots the raw JMS and MS data as a scatter plot, and shows the predicted gradient. It also shows a time series of raw JMS data, raw MS data, and also the scaled JMS data which hopefully follows the raw MS data very well. This may be quite tricky if there is only noise, but in such a case it is not a real problem, as its only noise after all. The get ratio button shows the ratio used when scaling up the m/z selected in the box, which is displayed as a single value in the panel, or as a graph if it is made time dependant.

The time dependant ratios selection box is to allow a different ratio to be calculated for different periods. To use this feature, tick the checkbox, and add a period to the wave by entering the date and time (in the appropriate format...dd/mm/yy hh:mm or mm/dd/yy hh:mm) then click add. To view all the points used click edit. The start and end points are omitted, so only "break points" are display in the wave. Remove will remove the point which is entered in the set variable display on the panel, if it exists in the wave, (the times must be identical).

The data type we always use is JMSDIFF, this must always be set correctly. If you use mssavg there may be a bug, as I have never ever looked at avg data and so cant test this extensively.

The JMS time series tab does the same as James' MS time series tab for MS data. You can choose whether to apply Airbeam corrections or not, which m/z to plot, whether to plot raw JMS data (jmss), raw MS data (mss), or scaled JMS data (jmssmss) which is imported to the ms waves. You can also recalculate the Airbeam correction wave using this new and improved JMS data that is imported to the MS waves.