Interactive comment on "Analysis of COSIMA spectra: Bayesian approach" by H. J. Lehto et al.

Anonymous Referee #1

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General comments:

The subject of the manuscript is very interesting because it leads the way to a possible automatic evaluation of mass spectra. This would be very useful for all TOFSIMS users because data evaluation can often take a lot longer than acquiring the data and is a major time sink. The introduction to the subject is detailed and informative but the result section seems rather a bit short and in some points misleading.

The manuscript is mainly concerned about single/double peak evaluation despite promising "the whole spectrum" in the abstract and this is where the manuscript falls short in my eyes. From the abstract I expected to see a full spectrum analysis and comparison with traditional methods like in Stephan T. (2001, TOF-SIMS in cosmo-

chemistry. Planet. Space Sci. 49, 859–906) for better judgment if this approach is actually worth it. Stephan also describes a peak fitting routine (although only for isotope rations but this could be extended to elemental ratios) which seems as promising as the Bayesian approach to me. Therefore a comparison of these two approaches would be helpful.

Specific Comments:

Section 4.3 is entitled Simulated Data but actually seems to mix simulations and real data and is therefore confusing. It would be better to keep the real data and simulated spectra separate in the result section.

The discussion of the two line case in section 4.3 fits better into 4.4. The discussion also falls a bit short as only total ion counts are discussed as being close to the starting point when counts for individual peaks are actually far off. The Bayesian method doesn't seem to work any better than a traditional approach marking peak limits and backgrounds. A better comparison with a traditional approach might be helpful here.

Page 578, lines 5-6: Surely the b term is determined by the mass resolution and not the mass resolution by the b term. And yes, every instrument/mass spectrum yields better results if the mass resolution is higher but you can't just increase the b term to achieve this.

Section 6: I'm not sure why the authors assume that in conventional analysis the background is ignored. Yes, some people might have done so and therefore skewed their results but by not ignoring the background, it's possible to gain good results using conventional methods, so it's not clear to me why the Bayesian approach has any advantage here?

Technical Notes:

The manuscript could do with some proof-reading. Some paragraphs especially in the introduction seem well written in contrast to some in the result section which have most

of the typos. I listed the ones I found below but this list is probably far from complete. There are also some very minor specific comments in here.

Page 567, line 12; recorded Page 576, line 13: AMD Page 576, line 19: "line parameters line" doesn't make any sense Page 577, line 1: shown Page 577, line 6: of or in Page 577, line 12: 5775 Page 578, line 1: such as Page 580, line 23: observed Page 581, line 1: I guess these are the mass calibration parameters a and b. Not sure why they are just called scaling parameters which seems rather confusing. Page 581, line 20: 13C+ Page 581, line 20-23: This sentence needs extending. It's not really understandable in its current form. Page 582, line 2: its Page 582, line 5: of Figure 3: That should be a separation of 6 bins and 4 bins respectively, not 6 and 6. Figure 4: The mass difference of these given masses is 0.027u.

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