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Atmospheric Measurement Techniques Discussions

Interactive comment on "PTRwid: a new widget-tool for processing PTR-TOF-MS data" *by* R. Holzinger

Anonymous Referee #2

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The manuscript is presenting a new tool for processing of PTR-TOF-MS data. PTRwid will help PTR-TOF-MS users to reduce the time needed for analysis of their measurements, which will be of great value for all measurements that exceed a couple of hours. The modular structure of this tool is user friendly, as it allows the user to process the data to any stage that is required or to ad tools. A publication in AMT would give the interest group the opportunity to get to know this tool, understand its functionality and facilitate the initial use of the tool, leading to an increasing number of users. The style of the manuscript is similar to a manual. This impression is mainly caused by figures 1, 7 and 10 (see suggestions below). In terms of peak integration it is not clear, if the peak/integration borders are adjused for each spectrum or if constant settings based on the sum spectrum are used. For highly variable compounds the signal intensity

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can vary substantially and the broadness of the peak changes. Signals of high concentrations could exceed the set borders of the sum spectrum. How does the peak integration deal with background/zero air measurements? Please find a further comments and remarks below.

Specific comments:

Line 20, page 1634: Why is a threshold of 8 σ used for the peak detection? Using the LOD (3σ) or LOQ (10 σ) seems to be a more obvious choice. Line 15-17, page 1635: The signals of H3O+ (19.018 Da) and H2O.H3O+ (37.028 Da) often show effects of saturation so that the signal is cut off and the highest data point does not necessarily correspond to the peak maximum. Therefore different (not massively) time bins would be associated with the H3O+ and H2O.H3O+ mass, respectively. Is this effect taken into account or can be neglected, since the range is small enough? Line 2, page 1637: Are the parameters yielding to the best match transferred automatically for the further analysis? Line 7, page 1640: What is the origin of the thresholds for DpB_sm of 0.55 and 5% of the maximum value? Line 10, page 1642: Usually a default value of 2x10ˆ(-9) cmˆ3 molˆ(-1) is chosen (e.g. (Holzinger et al., 2010). Can the default value for the reaction rate be changed and set individually?

Figure 2: The orange and the red line do not differ much and the different red markers are hard to distinguish. It would help the reader to pick up the details of this plot (upper panel) more easily, if more different or contrasting colours would be used. Figure 3: As the highest two peaks exceed the others in intensity by far, they are hardly visible. A break in the y-axis or an enlargement of the lower range could help here. The y-axis labelling for the lower three panels is too small. Figure 8, lower panel: Low contrast in colours (blue, black, green). Especially in a print out it is hard to differentiate between the black and blue markers. A clearer presentation regarding the colours would be appreciated. Figure 10: The order of the headers is not matching the displayed values. Values for mean and median are not displayed. Values following the ion's formulas are not explained.

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Structure:

As there are a couple of appendices, they should be ordered the way they are referred to in the text to provide a clearer structure. At the moment Appendix D is referred to first (line 20, page 1632), followed by A, B and C. The single procedures are explained later in the text in Section 2.1.3, so a reference to Appendix D is not useful before that section and could be removed on page 1632. Figures 1, 7 and 10 do not provide additional information to the text. The functionality of PTRwid can be understood just from the text. However, they are still useful for a future user of the tool, so I would recommend to integrate them into the appendix. Lines 13-18, page 1630: Very long sentence. Last part “the ions to be monitored do not need to be selected beforehand” as (iii) or separate sentence.

Technical corrections:

Line 14, page 1633: "... works on files that that contain ...". Line 7,8, page 1638: unclear structure of sentence, instead e.g. “...all peaks with a maximum signal within the following range:...”. Line 21, page 1639: "... the bin with increases...". Line 1, page 1642: "... of ions trough the TOF ...". Line 1, page 1645: "... the das phase inlet ...". Line 3, page 1647: "...on the SumSpectrum; which" (replace ; with ,). Lines 14, page 1647: too many commas, which are causing confusion. A suggestion: “(ii) a tool to create plots such as van Krevelen diagrams and presentations of desorption thermograms or carbon oxidation state, which...”. Figure 2, line 4: "The range ... is indicated by a horizontal red lines ...". Figure 9, line 8: "... the das phase inlet ...".

Reference:

Holzinger, R., Williams, J., Herrmann, F., Lelieveld, J., Donahue, N. M., and Röckmann, T.: Aerosol analysis using a thermal-desorption proton-transfer-reaction mass spectrometer (td-ptr-ms): A new approach to study processing of organic aerosols, Atmos. Chem. Phys., 10, 2257-2267, 10.5194/acp-10-2257-2010, 2010.

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