Faculty of Engineering and Sustainable Development

User Interfaces in Liquid Chromatography-Mass Spectrometry

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User Interfaces in Liquid-Chromatography-Mass Spectrometry
- a Case Study at Stockholm University
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Abstract
This thesis presents the issue of user interfaces in Liquid chromatography-mass spectrometry (LC-MS), the difficulties in their use, and what we think could be done to alleviate these difficulties. The project came about as a result of complaints from students at a chemistry laboratory in Uppsala. Case studies of the laboratories in Stockholm University and Karolinska Institutet were made in the form of interviews, questionnaires, on-site visits, and literature studies. Combining this work with our knowledge in computer science and visualization, we investigate the ramifications of user interface problems in this area as well as our proposition for solving them. Our study showed that there are unaddressed issues with interface usability and the handling of user feedback, and that there is a need both for further research and bolstered efforts to alleviate these issues.
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1 Introduction

1.1 Background

The original idea for our research came from a chemistry student in Uppsala. He voiced concerns about the user interfaces involved in his field: Liquid chromatography-mass spectrometry (LC-MS). This is a technique in analytical chemistry that combines physical separation of liquids through liquid chromatography, with mass analysis via mass spectrometry [1]. The field of chemistry where LC-MS techniques are widely in use is called proteomics and the goal for proteomics is quantification of the proteins in different complex mixes.

We thought the application of computer science to another field, especially one where it may not normally be given much attention, might make for an interesting topic for our thesis. Using the complaint of this Uppsala student and his peers as a starting point we pursued contacts at the chemistry departments at two separate institutes: Karolinska Institutet (KI) and Stockholm University (SU). Their different work environments, specifically with regard to user interfaces, allow us the opportunity to keep a wider perspective when examining user interfaces in LC-MS.

LC-MS has an important place in analytical chemistry because, among other things, the technique is used by medical science researchers in the investigation of drugs and complex processes in medicine. The two laboratories under focus in our investigation provide good examples of this kind of research: at KI they are researching specific cases of cancer mechanisms, and early detection and prevention of Alzheimer's disease. At SU they are doing research on neurotoxins, and the impact of certain substances on the environment and the atmosphere.

In this kind of work environment the precision and smooth operation of the expensive equipment involved – specifically mass spectrometers – is of paramount importance. As a consequence this is where most of the attention from instrument manufacturers is paid. However, students and others working with LC-MS still have to regularly use interfaces during the conducting of experiments; as it turns out, there are issues with these interfaces that haven't been prioritized or explored very deeply. That is where we come in.

1.2 Research Focus

Of the two laboratories that we will investigate, the one in Stockholm University will be the main focus. Here the software is included with the equipment from the manufacturer. This stands in contrast to the setup at Karolinska Institutet, where they use custom software programmed by an employee at the lab itself; the implications of these differences will be explored in-depth later.

The value of the applications of LC-MS is itself a testament to the value of anything involved in its process, at least any aspect that cannot be considered trivial or already solved. It can be shown that neither of these is true for user interfaces: for one, they are an inextricable part of the workflow when conducting experiments; further, as we will demonstrate, there are actual and specific problems that affect the efficiency of the lab work.

Figuring out precisely what problems students and researchers are having with the user interfaces constitutes a major part of our work, but before going into detail about those, we shall set out to learn more about these locations.

Our recommendations regarding the user interfaces will be stated based on our research findings, established guidelines for interface usability, knowledge of the human visual/perceptual system and how that pertains to interfaces, and the valuable discrepancy in the user experience that we have observed between KI and SU.
1.3 Research Objectives

The general objectives of our research are thus:

1. Find out what the students’ difficulties with the user interfaces are, if any.

2. Discover the sources of these difficulties.

3. Propose recommendations for improvement, if possible.

As detailed in subchapter 1.2 above, we hope to be able to recommend certain concrete adjustments and amendments to the interfaces, and suggest directions for further research.

1.4 Value of this research

We believe that the main value of our research is as follows: By doing an investigation in an area that, to our knowledge, has not seen much work done from this particular angle, we hope to highlight issues that might otherwise remain undetected or unaddressed. Furthermore, we think this could highlight this area as interesting for other researchers (and perhaps developers) with more time, expertise, and resources.

In any case, we think there is value in giving attention to an aspect of computer science as it is encountered in a different field, in this case analytical chemistry. Subdisciplines of computer science are utilized in many otherwise unrelated fields, and they are not always given the same attention and care as when they are dealt with in directly IT related businesses. Computer science should, in cooperation with other disciplines, be able to serve, support, and contribute to the solving of problems of serious demands in science these days:

“The sizable interdisciplinary boundaries make the communication problem challenging, but they also indicate a great need for improvements in visualization techniques due to their potential to provide a common ground that specialists in many disciplines can understand. The nature of the problems and of the solutions we have seen to date suggest that successful solutions to the open bioinformatic visualization problems will frequently prove to be complicated, ad hoc, and highly problem specific, much like the biological systems themselves. This should not mean, though, that we have to start from scratch with each visualization project we encounter.” [2, page 16]

1.5 Chapter Structure

* Chapter 1: Introduction

This chapter gives the reader a background of the field of LC-MS and what it is used for; this serves as a clue to why our own research is useful. After an outline of our research focus and methods, tying back to the initial statement about the applications of LC-MS, follows the stated value of our research as we see it.

* Chapter 2: Theoretical background

This chapter contains a literature review, focusing on user interface guidelines and user interfaces in analytical chemistry, which is used to confer theoretical credence to the research.

* Chapter 3: Environments
Here we give a more detailed background on the two environments we have done case studies for: the respective chemistry departments at Karolinska Institutet and Stockholm University.

* Chapter 4: Research Methods

In this chapter we describe in detail our choice of research methods, why we used them, and how we formulated them. The structure of these methods was chosen based on the work we expected to do, and the requirements of the environments under study. This ties back to the previous chapter, and also onward to the actual results we obtained using them.

* Chapter 5: Case Study Results

Here we present the concrete results of our investigation of the laboratories at KI and SU. Interviews, questionnaire responses, and information obtained via email, documentation, or conversations are summarized for an overview of our findings. This chapter also contains descriptions of workflows in the laboratories (Figures 1, 2, and 3).

* Chapter 6: Discussion

Following chapter 5 is our discussion of the results and what we think should be done based on them.

* Chapter 7: Conclusion

Here is the final summary of our findings, reasoning, and recommendations.

* References

References to literature in various forms are contained here.

* Appendices

Available in this chapter are transcripts of all recorded interviews and questionnaire results, to formally support our findings and arguments.
2 Theoretical Background

Two different perspectives on user interfaces are presented in this chapter to provide an established standard by which to evaluate them, and to apply knowledge to our specific area of interest.

2.1 General guidelines for evaluation of user interfaces

Although applications of graphical interfaces in specific fields come with their own requirements and conventions based on the needs of those fields, several sets of general guidelines for interface design have been proposed. Two of them are listed and compared below; for the sake of brevity the original descriptions of the points within have been omitted where the point titles were deemed self-explanatory, or otherwise paraphrased in shortened form.

Ben Schneiderman's "Eight Golden Rules of Interface Design" [3]:

1. Strive for consistency: Consistency in terminology, commands, and sequences of actions.
2. Enable frequent users to use shortcuts.
3. Offer informative feedback: Feedback severity should be based on the rarity and importance of a user's action.
4. Design dialog to yield closure: Procedures should be organized so as to have a distinct beginning, middle, and end, with the end being clearly signalled so that the user can consider the task accomplished and move on to the next one.
5. Offer simple error handling: Disallow the committing of errors where possible and otherwise give clear indications of the errors' nature and solution.
6. Permit easy reversal of actions.
7. Support internal locus of control: Users should be in control, not respond to frequent prompts from the program.
8. Reduce short-term memory load: The limitation of human information processing in short-term memory requires that displays be kept simple, multiple page displays be consolidated, window-motion frequency be reduced, and sufficient training time be allotted for codes, mnemonics, and sequences of actions.

Jacob Nielsen on his Ten Usability Heuristics: 'These are ten general principles for user interface design. They are called "heuristics" because they are more in the nature of rules of thumb than specific usability guidelines.' [4]

1. Visibility of system status: Keep users informed about what is going on in the system.
2. Match between system and the real world: The system's language and appearance should be intuitive to users.
3. User control and freedom: Allow reversal of mistakes; support undo and redo.
4. Consistency and standards: Users should not have to wonder whether different words, situations, or actions mean the same thing. Follow platform conventions.
5. Error prevention: Prevent errors outright or present users with a confirmation prompt before making decisions that might lead to such.
6. Recognition rather than recall: Keep objects, actions, options, and instructions visible and readily available, and do not require memorization of dialogues past their span.
7. Flexibility and efficiency of use: Accelerators - unseen by the novice user - may often speed up the interaction for the expert user such that the system can cater to both inexperienced and experienced users. Allow users to tailor frequent actions.
8. **Aesthetic and minimalist design:** The user's capacity for information is limited - if info is included, make it count.

9. **Help users recognize, diagnose, and recover from errors:** Error messages should be expressed in plain language (no codes), precisely indicate the problem, and constructively suggest a solution.

10. **Help and documentation:** When necessary, provide documentation that features concrete instructions without being too long.

Evidently there is some overlap among the suggestions of these authors. Still, they each provide unique advice, notably points 4 and 7 from Schneiderman's list and points 2 and 10 from Nielsen's. Schneiderman's words on "closure" seems to relate to his own and Nielsen's recommendations not to overload the user's short-term memory. This point could be interpreted to say that enabling the user to decidedly put a given task behind him frees up mental resources, both in terms of memory and concentration, for the next step in a procedure.

Interestingly, Nielsen argues for a lack of external documentation in such cases where one can get by without it. It would be easy to argue that some systems are bound to be too complex to be supported by context-sensitive help alone. Presumably the LC-MS devices belong to this category, but it does bring into question the quality of the admittedly lengthy documentation that has been confirmed as being a main source of complaints from the students who have to learn it.

The combined rules from these authors will be used to assess any specific issues found in the user interfaces.

### 2.2 Software and User Interfaces in LC-MS

According to Hu Zhou et al.[5], the development of good algorithms and appropriate software for LC-MS is a big challenge, and is an area that needs further modifications. Improvements in that area can lead to a better study process for the students and more effective research flow for the scientists who work with LC-MS.

Liquid chromatography-mass spectrometry is a very widely represented topic in the scientific community. In analytical chemistry LC-MS takes an important place because the technique is used by medical science researchers in the investigation of drugs and complex processes in medicine:

> “The goal of proteomics is to identify and quantify all the expressed proteins expressed in a biological system under specific conditions. Mass spectrometry (MS) has developed into the method of choice for achieving this goal. The success of MS as a powerful analytical technology for biomolecule analysis is due to several technological accomplishments including the development of efficient protein ionization methods and advances in mass analyzer hardware.” [6]

The focus of our search was the actual software used for LC-MS, the interfaces used in that software, and methods of visualization of LC-MS data. We compared articles describing different software such as VIPER (Visual Inspection of Peak/Elution Relationships), Decon2LS [7], msInspect, EPI Suite software [8], and mzMine [9], and found some key points that appear to be common for all types of software.

LC-MS data needs well organized 3D representation. According to Bellew, Coram *et al.* [9] 2D is not the best way for analysis of LC-MS data. Due to the complexity of the data obtained from LC-MS there is an obvious need for graphs and plots showing the different phases of the process; the user should be able to choose the parameters for the axis of the plots and so on. Whereas the msInspect software features the option to zoom a 2D image in and out, VIPER on the other hand allows for changing the colors of desired objects. VIPER and msInspect use 2D representation, and according to Linsen *et al.* [1], analysis of 2D plots does not give a complete understanding of the data received from LC-MS; the 3D representation
model introduced by them allows “global understanding of the absolute and relative intensities.”

Although these techniques seem to be very innovative and feature high performance, the authors [1] cite Corral and Pfister who created a similar method for visualization; they modified the method that Locasso and Hoppe invented. This means that the area of LC-MS is developing rather intensively; there are various scientists who have similar ideas and they present them in the form of software or new methods for visualization. This is a beneficial trend, but for the people who deal with LC-MS it can be a problem since significant changes in the software and visualization techniques can induce slow workflow and ineffectiveness.

Previous research on proteomics and human-computer interaction together lead to a conclusion, that even small changes in the user interface can lead to significant change of the scientists workflow [10].

Different laboratories work with different hardware and software. While the general principle is the same in terms of chemistry, it can be rather confusing to get used to and understand software that is developing dynamically. The majority of articles taken into account were written in the year 2006 and we can assume that during the last 6 years new software has appeared in the market of analytical chemistry software.

2.3 Summary

Evaluation of LC-MS software and analysis of the visualization methods used in different software used for this technique will lead to determination of the particular problems, and proposals for possible solutions. Different software was tested and compared in order to understand the needs for further development. Interfaces and visualization of the data are the critical features when it comes to usability and effectiveness of the software in the field of analytical chemistry; this is why better software leads to better workflow for scientists and students who deal with LC-MS technology.

The results of this literature review will help us mainly in accomplishing our first goal, since they grant us an established view of evaluation of user interfaces. Although the "8 Golden Rules" and "10 Usability Heuristics" are quite general, we believe they will apply in large part to our particular problem, and that most of them will find expression in one manner or another.
3 Environments

While the two laboratories we have visited are basically similar in that they both work with LC-MS, they do feature differences that affect the way their staffs handle user interfaces. Here we will examine these environments separately and then present a summary of the differences that are the most important to us.

3.1 Karolinska Institutet

At Karolinska Institutet there is a department for Medical Biochemistry and Biophysics, with a number of laboratories for specific experiments. For the process called liquid chromatography-mass spectrometry there are separate laboratories and special hardware that performs the procedure of LC-MS. Mass spectrometry machines work with biological samples of complex protein mixes.

The process is initiated by inserting samples into the machine. It takes approximately one hour to process one sample, so if the experiment is a large one with numerous samples, the procedure is rather time demanding. The output is in the form of so-called raw files that are to be used in other software for analysis. These machines can be used in various ways depending on what kind of experiment needs to be performed and what kind of data is to be gathered. LC-MS is widely used in pharmacology and medical science. In the MS laboratory at Karolinska they use machines manufactured by Thermo Orbitrap.

Examples of recent projects are investigation of anti-cancer drug development, and early detection of Alzheimer's disease. People who deal with these machines are scientists and PhD students. The procedure of processing the samples does not require much user interaction beyond placing the samples into the mass spectrometer and pushing the “Go” button. As previously mentioned, LC-MS is a very time demanding process, so while it is running, scientists have time to do something else. When the hardware process is over the results have to be analyzed and interpreted.

At Karolinska they use a piece of software called Quanty which at present is written and maintained by Yaroslav Litvinsky, a programmer at Karolinska University, who developed the software for these particular machines. The program runs rather quickly -- the process of interpretation is 10-15 times less than the process of getting the sample out of the mass spectrometer -- and gives accurate results, but involves user interaction at different stages during run-time. The output of this software is a very large table with a list of proteins in samples, and specific numbers for each protein in a sample. The table does not give any interactive reports, so the user must himself transfer the data to external programs – MS Excel and the analytical software programs Simca-P+ and Perceus – to acquire correlation graphs of the protein/peptides dependence that influenced the given result.
3.2 Stockholm University

Stockholm University has many specialized departments. The one we have visited is for Medical Biochemistry and Biophysics. There are Bachelor, Master, and PhD students, and scientists who work with environmental studies and research. Of interest to us were the students working with LC-MS. These people work with mass spectrometers and analytical software in a lab.

The process begins with installation of samples into the auto-sampler, and preparation of the hardware by inserting the instruments and parts of the pipeline that will be used further. When the hardware is organized in an appropriate way it has to be adjusted through the instrument control software to set the parameters (molecular weight) of the scan range, the depth reached by the sampling needle et cetera.

The mass spectrometers used here are from a company called Thermo Finnigan. The software for analyzing results obtained after the actual process of separation of the proteins in a sample is also provided directly from the manufacturer. When problems occur, students and scientists can always contact the manufacturer to get help and support straight from the source.

A piece of software called Xcalibur is run straight after the hardware is finished with its work. To be able to get the desired result the user is actively involved during the analytical software workflow.

The analytical chemistry department focuses on organic and bio analytical chemistry. Their research area includes topics such as carcinogens in flame retardants, detection of allergens, environmental analysis, and proteomics.

3.3 Differences between work environments

Organizationally, the lab at KI is under greater pressure to deliver tangible results of their research, whereas the work going on at SU is more educational in nature. One could surmise that the stricter requirements at KI extend to the daily operation of their user interfaces as well, which brings us to the central difference between the two labs - - at least as far as we are concerned: KI uses custom software written and maintained by one of their employees, whereas SU uses software produced by the hardware manufacturer, and which comes bundled with the equipment. It is not a new occurrence in the realm of scientific work to have their own developed software which suits their purposes [6]; KI is an instance of this.

When it comes to problem solving or support, at KI the only source is the programmer who created the program. Meanwhile at SU they can contact the manufacturer directly and ask for help. In some ways it is convenient to have a developer on location, because he knows the program from its inception and can fulfill the needs that can arise during the work. But it can cause inconvenience if there is no possibility to access him. At KI the amount of samples and sample sizes (currently over 100GB of raw data for each full scan) are bigger than at SU; that is the reason why mistakes occurring during the process at SU do not cost as much as they do at KI.
4 Research Methods

We started by uncovering the users’ views on their software, first via email correspondence, then through visits to the laboratories where handed out questionnaires and conducted interviews. These are our main research methods.

Most of this work was done at SU, and fortunately they have been cooperative in allowing us access to the lab and the students there. This is a broad objective that encompassed a multitude of activities: asking initial questions in emails to laboratory staff, discussing our research approach with the supervisor, consulting technical documentation, carrying out interviews and questionnaires, and more.

4.1 Introduction

Our first research objective is to find out any problems chemistry students may have with their user interfaces. This constitutes the central part of our investigative activity. While the obvious thing to do in this case was directly soliciting the students for their views, we had to go about this in such a way that the information we obtained is both valid and reliable.

This chapter will describe our choice of research strategy and methods, why we chose them, and how we implemented them for our specific purposes.

4.2 Research Strategy

Overall our research is a two-part case study of the Department of Medical Biochemistry and Biophysics, Physiological Chemistry I at Karolinska Institutet (KI), and the Department of Analytical Chemistry at Stockholm University (SU), with the latter being the main location. The reason for this uneven division of focus is the fact that the lab students and workers at KI use their own software, which allows them greater facility to address their concerns. We include KI in our research because there will be a salient point to make about this difference in the discussion of our results.

In deciding whether to perform a narrower case study or spread our attention across more laboratories, we chose the former option based on the following reasoning: Although investigating a greater number of work environments could make the case for generalizing the results of our research findings more plausible, the attempt would not be worth jeopardizing the accuracy of the data collected at each site, given our limited resources and time.

As mentioned in the introduction, the "first indication of trouble" came from a student in Uppsala. To preserve objectivity in our research we searched for other laboratories where our contacts are strictly third-party.

The staffs at both locations are small enough to eliminate the need for any sampling method. All available students at SU were given the questionnaire and interviewed.

4.3 Data Collection

4.3.1 Overview

We observed the working process of the LC-MS procedure, and talked to students and professors who work with it. The analytical chemistry department is rather large but there are only a few people who work with LC-MS.

Our main method for collecting data was the distribution of a questionnaire, followed by interviews. The intent in this setup is twofold: the questionnaire gives us a standardized form of questions and answers that can be collated into quantifiable (though limited given the small population) statistics while the interviews allow back-
and-forth discussion; the progression from questionnaire to interview makes it possible to ask for clarification of issues that have been previously brought up.

### 4.3.2 The Questionnaire

The questionnaire was prepared in advance based on our observation of the work flow and the software that is used to operate the results from the liquid chromatograph, the machine that does the physical work of separating proteins in liquid mixes.

The questionnaire contains 10 questions about the software interface, such as what users like about it or what can be problematic with it, and we also asked what they wish to be developed to make it easier to work with and more user-friendly. We constructed our questionnaire based on the manual for the software [11] and observations that we made during the first visit at the LC-MS laboratory.

We used the book Research Methods for Human-Computer Interaction [12] for the general structure and flow of both the questionnaire and interview. We were also inspired by a similar project in evaluation of usability of a web based application interface, where they used the methods and approach with questionnaires in order to gather user feedback [13]. We believe this approach helped to give us a rather full overview about user opinions and spotting common patterns of complains about the software interface. For information about what questions to ask and what should be investigated, we found very thorough hints by Carla Merrill and Diane Feldman [14].

We attempted to formulate our questions in such a way as to not affect the respondents' answers too much, and we tried to keep suggestions of our own ideas to a minimum to get as much of their own opinions as possible. However, these considerations had to be balanced against the need for some direction from our side, as the respondents are not necessarily acquainted with our field and so might fail to mention, in open questions, alternatives that may very well apply to them. The questionnaire form can be found in Appendix I.

### 4.3.3 The Interviews

Some of the interview questions are shared with the questionnaire, or are expanded versions of them. In these cases we asked why the respondents previously answered in a certain way, or prompt a clarification of what exactly they meant by choosing a given answer.

The interviews were conducted by Valentina with one participant at a time, while Emil took notes and made sure the relevant topics were addressed. Regrettably we did not have the opportunity to assemble a focus group to complement these interviews, but we were able to hold shorter informal discussions with more than one student at once.

All interviews were audio-recorded and transcribed. Transcriptions with anonymized participants can be found in the appendices of this document. The interviews were conducted in English and the transcripts edited for the sake of clarity, brevity, and what we believe to the best of our ability and judgement to be the accurate portrayal of the participants’ opinions and statements.

### 4.3.4 Summary

This method of collecting the data was chosen because, in our opinion, it is the best way to get user feedback and a better understanding of the existing problems:

"Depending on what we are investigating, sometimes it is useful to start with a questionnaire and then, for example, follow up some specific points with an experiment, or a series of interviews, in order to fully explore some aspect of the phenomenon under study." [12, page 17]

One of the objectives of our thesis is to find out what the problems are and of what kind. That is why we interviewed the group of people who are using the
analytical software for the LC-MS procedure, and can give us real and relevant data that we can use in our proposal for development, which is another of our objectives. In addition, SU is our major case study and, as was mentioned before, there are just a few people (6-10) who work specifically with LC-MS. That is why we interviewed them in detail and gave the questionnaires containing the questions connected to what they specifically deal with.

4.4 Data Analysis

The relatively small amount of quantitative data from the questionnaire is in the form of yes/no and 1 to 5 scale answers, and did not take long to compile. A less clear issue is how to quantify the latter type. We suspect that, in themselves, these answers won’t be useful beyond allowing us to claim in general terms that the students are so and so satisfied or displeased with certain features. But we expect them to give us clues for the follow-up interviews, which is one of the reasons we structured our research this way.

The qualitative data is ultimately of greater interest to us. That is where we will find specific descriptions of existing problems, and suggestions or wishes for improvement. This data is also what enables us to make our evaluations against Schneiderman’s and Nielsen’s rules, since it states problems in the more definitive form of the users’ actual experiences, rather than numbers that are difficult to translate into problem descriptions without involving too much of our own interpretation. In other words, it is easier to get an accurate idea of a problem’s nature and severity through words than a simple number.

4.5 Limitations

There are always some kinds of limitations that can constrain the results and change the whole process of the thesis. Sometimes they appear due to time limits, or the specific problems of the area of the research, or due to some formal limitations. Although we planned the research strategy very carefully, we want to acknowledge the limitations we encountered on the way.

Firstly, the area of LC-MS is rather narrow, so even though the department of analytical chemistry is big, only a few people work with the software we are interested in; to be precise, about 8 persons. That is one of the reasons we chose to do our research at two places, Karolinska Institutet and Stockholm University, to get a better understanding of the problem. We are wary of trying to generalize results too much; this will need to be the task for possible future research. We made questionnaires and recorded interviews, where we ask for the personal opinions and wishes of the students, so a question is whether these problems are experienced by every student with a similar occupation, or if they are specific for this environment and this student.

The software we are investigating is operated on Thermo Fisher hardware and provided by the manufacturer, whom we tried to contact but did not get any response from. That could be very useful information because both KI and SU use their hardware, and description of the software and support provided from the manufacturer could be a valuable contribution to our thesis, but unfortunately it was not possible to reach them.

Not all students could participate in both the questionnaire and interview, but we believe that we were able to gather most of their views regardless.
5 Case Study Results

Here we present the findings from our two main methods of data gathering: the questionnaire and interviews. For the questionnaire the form with questions is provided, along with the answers in a table. Interview replies are treated per individual student; the students are referred to as "Student A", "Student B" etc. instead of their actual names. These students are from Stockholm University and are studying on the Master’s or PhD level.

We also provide schematics of the workflows of the relevant user interfaces at both Karolinska Institutet and Stockholm University.

5.1 The Questionnaire

As was mentioned in chapter 4 we distributed a questionnaire to students who work with LC-MS in the department for analytical chemistry at Stockholm University. In this questionnaire there were 10 questions regarding the interface. We received 6 completed questionnaires and even though the sample size is small, we can see the pattern in the answers:

<table>
<thead>
<tr>
<th>Question/Student</th>
<th>Student A</th>
<th>Student B</th>
<th>Student C</th>
<th>Student D</th>
<th>Student E</th>
<th>Student F</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q1</td>
<td>2</td>
<td>2</td>
<td>3</td>
<td>2</td>
<td>4</td>
<td>3</td>
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<tr>
<td>Q2</td>
<td>2</td>
<td>2</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>2</td>
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<tr>
<td>Q2 a(if Q2 = 1)</td>
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<tr>
<td>Q2 b(if Q2 = 2)</td>
<td>a, b</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
<td>a</td>
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<tr>
<td>Q3</td>
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<td>2</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>Q4</td>
<td>a</td>
<td>d</td>
<td>a, b</td>
<td>d</td>
<td>c</td>
<td>b</td>
</tr>
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<td>2</td>
<td>5</td>
</tr>
</tbody>
</table>

Table 1. Answers to the questionnaire

The answers here are numerical for questions using the 1-5 scale for the single answer given, and a letter for questions with a number of alternatives. Question 2a and 2b depend on whether the answer to question 2 is Yes or No.

It is seldom that they have completely different opinions; for the most part the majority of students have the same or similar opinion. We believe that the answers given by students depend on their experience and how long they have been working with LC-MS software overall. Above is the table with answers to all the questions. The questionnaire template can be found in Appendix I.

5.2 The Interviews

These points are a condensed report of those views expressed in the interviews that are directly relevant to our research findings. For the full transcripts consult Appendices II through VII.

5.2.1 Student A

- Found it rather easy to deal with the work process in the beginning, thanks to the assistance by a supervisor.
- Needed about 1 month to feel comfortable with the process.
• Did not like the way the software quantifies peaks, and would instead like to do it manually.
• Would prefer customizable tables, to integrate peaks and perform calculations on their own.
• Valued visualization at 3 and precise numbers at 5, arguing that precision is more important than presentation.

5.2.2 Student C
• Did not find it particularly easy at first, at least in part because of that particular instrument’s and software’s age, but remembers being accompanied by PhD students who would offer help.
• States that they went through the most important parts in lectures.
• Claims that there were several phases to learning the software initially but that, thanks to the help received from PhD students, it didn’t take that much time to get used to it.
• Has a specific complaint about the user interface: "In each scan, I scan different transitions. Each transition gives me 1 peak. For example, in my scan I have 4 transitions; I should have 4 peaks at the same time. The software separates the 4 peaks into 4 windows. I want them all in a single window, which would make it clear and easy to show in publication. Some instruments do that and then it's very good."
• Thinks it’s difficult to find explanations of specific concepts in the built-in help.
• Considers mistakes made during the process time-consuming to rectify, sometimes requiring a system restart.
• Considers graphical charts quite important.

5.2.3 Student E
• Consults the supervisor and manual when necessary, and did not typically find it difficult to work with the software at first, other than when running into certain problems requiring assistance.
• Has found computer science terms in the built-in help hard to understand.
• Finds there is a lack of shortcuts between different windows, and a lack of ability to use several windows simultaneously.
• Considers correction of mistakes risky since some processes hang the software if cancelled, and undoing data treatment requires closing and then reopening the data forms.
• Would like more options for graphical charts to visualize data; rated the importance of graphical representation 4, and accurate numbers 2, with the reasoning that the former helps give an overall impression of the data, and aids in making good decisions for the next step in the process.

5.2.4 Student F
• Found it very complicated to run tests in the beginning, due to an abundance of buttons and a lack of organization in the user interface.
• Needed one week of continuous work to feel more or less comfortable.
• Considers the optimization tuning of compounds the software’s strongest point.
• Thinks that window/page navigation is restrictive and unintuitive.
• Remarks that two-word searches in the built-in help yields results for each term separately, which necessitates a long manual search to find the right entry.
• Notes that buttons and icons are often cryptic, their meaning not being clear or explained.
Claims that trying to "Undo" a mistake such as starting a sequence without having put the vials with samples inside the mass spectrometer may result in having to restart the computer or the instrument.

Thinks there is too much dependence on mouse clicking and unnecessary amounts of navigation required to choose certain options for repeated tasks.

On the process of online chromatography: there is no option to view the chromatography for the previous sample when a new one is active. Updating large peaks requires manually closing and reopening parameters window.

Certain effectively mandatory steps are optional for no reason: wants them to be automated.

Considers graphical representation of data important, since Excel is available for working with tables.

On offline chromatography: updating it requires repeatedly pressing F5; there are no scripted or automatic updates.

Would like additional buttons for certain functions such as showing the area or the peak, not just integration.

5.2.5 Professor A

Considers free experimentation the best way for students to learn the user interface.

Considers accuracy of numbers to be of the highest importance for scientific research.

5.3 Workflows

During our visits to the laboratories we observed, and asked questions about, the specific steps involved in the work with Quanty and Thermo Finnigan’s software. Since there were no schematics available for these workflows in the instruction manuals or elsewhere, we have constructed them based on information obtained on-site.

5.3.1 Quanty workflow

- Set up an experiment
- Randomize the samples
- Insert blanks where needed
- Run the experiment
- Check the progress of at least the first sample
- Obtain .raw files
- Generate .mgf files
- Launch RAW2MGF program
- Select parameters

- Launch MGF2DAT program
- Merging individual .mgf files into a common .mgf file

- Launch Cluster MGF program
- Choose filtering parameters, file name

- Launch Quanty program
- Select .dat files obtained from the previous step plus initial .raw files

- Very large dataset in a table
- For further analysis, another software has to be used like MS Excel

*Figure 1. Workflow for Quanty*
Figure 2. Schematic structure of Quanty

5.3.2 Thermo Finnigan workflow

Set up an experiment
- Insert the samples into auto-sampler
- Optimize hardware settings suitable for particular experiment

Run the experiment
- Check that sampling needle started its task

Instrument setup
- Launch Xcalibur program and go to Instrument setup – See the screenshot ‘thermo_frontpage.png’
- Create a method for LC
- Parameterize gradient of the pump (time, flow rate, composition of the mobile faces in percents) – See screenshots ‘xcalibur_2_instrument_setup.png’ and ‘xcalibur_3_gradient_program.png’
- Save the method that was just created

Sequence setup
- Check that mass spectrometer is on “Load” mode, otherwise results can be wasted

 RAW2MGF program
 .raw
 Mascot
 MGF2DAT program
 Cluster MGF program
 Quany program
 .raw
 .raw
 .raw
 SQL
- Set parameters such as name of the sample, comments, path, instrument method, position, injection volume – See screenshot ‘xcalibur_4_sequence_setup.png’
- Online chromatogram is shown while the process is active

**Data treatment**

- To see the peak area after the experiment is completed, open chromatogram and smooth the graph
- Integrate the peak, maximize it to see the actual border (better to do this manually - auto integration often selects the wrong area) – See screenshots ‘xcalibur_5_display_option.png’ and ‘xcalibur_6_chromatogram_ranges.png’
- Choose parameters desired for display

*Figure 3. Workflow to setup an experiment on Thermo Finnigan software*

During the workflow the user is constantly involved and forced to control the flow of the experiment. Data has to be saved several times during the whole process in order to maintain the procedure and obtain the right results. A number of manual setups and available options make it hard for the user to maintain track of the workflow. If some small detail is missed, the whole process can crash. For new students this can be difficult, because it takes time to become familiar with the program.
6 Discussion

As a discipline, user interfaces are not directly related to the primary field in which it is applied here. Thus our initial supposition was that it may be a somewhat overlooked area. After having conducted email correspondence, telephone calls, and on-site visits, this has been confirmed in some important respects, though mainly so for SU.

Initial responses to inquiry were reserved, but after more interaction we managed to find more specific problems. Hopefully this will allow us to propose more specific recommendations.

6.1 Analysis of research findings

As an early look into the students’ relation with the software, the answers to the questionnaire seem only to present a presence of isolated issues rather than any major discontent with the work process as a whole. This indicates that the process as such is functional (as one would expect for such established and expensive hardware and software) but that there are indeed issues with the software that lead to inefficiencies.

This fact and its details are explored and confirmed as we investigate the findings from the interviews and informal conversations with the students.

6.1.1 Answers to the questionnaire

The students are generally satisfied with the initial learning curve of, and help with the software. We believe the presence of PhD students in and around the lab is largely to thank for this, since they are readily available for assistance and have knowledge and working practice of the software fresh in memory. Still, the answers make it clear that things could be better in this area.

Only two students use the paper manual, and only one of those stated that it contains information not found elsewhere. The software’s built-in help function and other students are the main sources of help. From our own reading of it we can tell that the manual is thorough, but dry, repetitive, and replete with repetition of cautionary advice; all of these make it less efficient than it could be for the purposes of referencing. In our own experience this appears to be a common problem with full length technical documentation. The students’ own replies point to its redundancy in the presence of other options.

The built-in help is probably not the sole or even main responsible factor for this, however, since it scored only average on usefulness; missing or cryptic descriptions of problems and terms are the primary offenders here. Incidentally, this mirrors our own experience with such help functions. But even if this problem is not unique to this software, it could stand to be addressed. One of the common problems is that a built-in help does not search for a phrase, it only gives a result for separate words and that makes the list of results very long and hard to parse.

Interface navigation is another area that was rated average. For some students this has to do with layout or flow of the interface; but none of them are outright unable to work with the program, so, as most of the answers indicate, the lukewarm sentiments about navigation stems from specific issues such as error/mistake handling.

Students rated numerical representation of data as more important than graphical representation, though the latter still received higher than average scores. They are also interested in having more graphical charts at their disposal.

Questionnaires gave us valuable facts and information, but to understand the reason why students think that way we interviewed them. There are more details about that in the next subchapter.
6.1.2 Responses from interviews

After collecting the questionnaires, we interviewed almost every student to get a better picture of the problem domain. We also interviewed associate professor Ulrika Nilsson who has great experience in this field, and gave us guidance and valuable hints about the software we are investigating.

The students’ interview answers were rather similar to each other; it is hard to understand the program in the beginning, and most of them were given help from a professor or students who have already been working with the program. That is also a reason why the majority of students do not utilize the manual for the software.

Complaints about the built-in help were mostly about inconsistency of the search function. It is not possible to search for combinations of words since the program will show separate results for the match with the first word and with second word, but not these words together. Thus finding required information is problematic and time consuming.

A majority of the students have some problems navigating through various windows of the program. Sometimes they have to have many windows open which leads to confusion and disorder in their work process. They have to close some windows and then go back to what they are working with now, and that can happen several times which is irritating and hard to keep track of. Correcting mistakes is another problem we got complaints about. If something goes wrong it is not possible to correct the mistake on-the-fly; the whole sequence or the process has to be canceled and started from the beginning.

Wishes for better data presentation include more customizable tables, and graphical charts. In the interview with Student G he stated a wish for automatic reports at the end of the process, which is not a feature that is present today. If a student wants to analyze the data he/she got, that has to be done manually.

6.2 Interface evaluation

Interface evaluation should be based on theories and rules; here we correlate Schneiderman’s rules and Jacob Nielsen’s theory about what good interfaces should look like with our findings.

6.2.1 Ben Schneiderman’s “Eight Golden Rules of Interface Design"

1. Strive for consistency: The interfaces are internally consistent, for the most part, but cross-system standardization is not as good as it could be, given the commonality of their features.
2. Enable frequent users to use shortcuts: Certain options, especially those that must be repeatedly activated, could use more shortcuts. The same is true for various windows when they need to be accessed in the middle of the work process, but the process that the students go through is mostly linear, so in general they do not need frequent access to past or future steps.
3. Offer informative feedback: Feedback about the internal processes in the hardware is mostly clear. Data presentation is a separate matter.
4. Design dialog to yield closure: This rule is generally followed by the software, but there are parts of the process that require unnecessary repetition.
5. Offer simple error handling: This is perceived to be one of the program’s weak points. Specific examples are offered in the results of the interviews, and we uncovered a few more during a later demonstration:
   • There is no default functionality to indicate or prevent a user from setting the depth reached by the syringe needle low enough so that it pierces and destroys a sample container, if a special insert is used
• There is no indicator in the software to tell whether the setting for samples is set to Load or Waste. If the user forgets to check the LED indicator on the hardware, samples may inadvertently dumped.

6. **Permit easy reversal of actions:** In LC-MS there are inherent limits to how many and what type of actions can be easily reversed, due to the nature of the scanning process. Still there are actions in the software that could be made reversible with lower cost in terms of time expenditure.

7. **Support internal locus of control:** In this program, users are the main initiators of action, so the program certainly adheres to this rule.

8. **Reduce short-term memory load:** Many of the activities done in the program are sequential and done in short steps, which helps prevent overloading of short-term memory. However, there are exceptions: Windows showing chromatograms are not consolidated when several are displayed at the same time; Methods for the MS operation (including settings such as scan range in molecular weight) must be manually saved and; Some options for peak detection must, if desired, be selected over and over again for every adjustment, since the program does not remember them. This invites user error due to frequent repetition. Selected options should be remembered by the program, and unnecessary user actions automated.

6.2.2 **Jacob Nielsen’s Ten Usability Heuristics:**

1. **Visibility of system status:** This is fulfilled to an extent, with some notable exceptions; See Schneiderman rule #5.

2. **Match between system and the real world:** The language used in the software makes sense to chemists, which is the sole intended group of users.

3. **User control and freedom:** See Schneiderman rules #5 and #6.

4. **Consistency and standards:** See Schneiderman rule #1.

5. **Error prevention:** This is related to rule #5 above. Nielsen specifically asks for prompts before potentially problematic decisions are made, and these have been shown to be missing for certain actions.

6. **Recognition rather than recall:** Mostly followed, though some users find various buttons and icons unintuitive.

7. **Flexibility and efficiency of use:** There is not much provision for altering aspects of the process that has to be gone through in the software.

8. **Aesthetic and minimalist design:** In software for LC-MS there is a need for many options and displayed features; if the program has any shortcomings here, they can be excused on those grounds.

9. **Help users recognize, diagnose, and recover from errors:** The program does not feature many error messages.

10. **Help and documentation:** See evaluations of the physical manual and built-in help.

6.3 **The aspects of custom software**

What implications could these differences have for the extent and nature of any problems experienced by their respective users? Our research results may shed some light on this. We know that the software at KI has been updated 17 times in the last 18 months; these updates were made by the original creator himself, who also works on location at the lab and is available for tutoring and instruction.

This close proximity with the one who is responsible for the software yields several obvious advantages: students can quickly get help from the foremost authority on the software; they can submit feedback directly to the source; adjustments are made faster.

But are there any potential dangers with this approach? Questions that come to mind are: What happens if the author of the software leaves his position at the
laboratory? Who has the rights to the software he developed? Who will manage updates, modifications, training, manual etc.?

As of yet, the program at KI has not been published, and so belongs to the author, with an exception: certain algorithms that have been used with permission from a third party source. Because of this, he is not certain of the actual legal status of the application’s ownership. There is a patent pending but they do not intend to turn the software commercial.

The author claims that, should he leave his position, someone else could be trained in two months to perform his work.

6.4 Handling of user feedback and experiences at SU

The setup at SU is more traditional: off-the-shelf hardware and software. This puts the responsibility for development, updates, security etc. solely on the vendor. The students only need to manage replacement parts for the hardware, though they occasionally receive visits by engineers from the vendor.

The biggest contrast in this area that we’ve observed between KI and SU is that there appear to be few or no provisions for the students at SU to voice suggestions about their software, and have them implemented or taken into consideration for future development.

Going by what the students have told us, there appears to be a disconnect between them and the equipment manufacturer regarding the software’s problems as the students see them; they do not agree as to the extent of these problems.

Could the following claim offered by Carla Merrill and Diane Feldman pertain to this?

“Companies have their reasons for not focusing on the user’s logic. The main argument is that users don’t know what they want, which means that the process of eliciting user needs is nebulous with no definitive end. It is far easier and more familiar to start with a list of requirements negotiated between marketing and development managers and then develop a plan to implement the list.” [14, page 51]
7 Conclusions

7.1 Research Objectives

In the beginning of our research we stated three objectives that we wanted to achieve. The first of them was to find out what the students’ difficulties with the user interfaces are – if indeed there are any at all. We found out that even though the software used both in KI and SU is functional and performs the jobs it is tasked with, there are a number of problems. Students have problems with built-in help functions, navigation through the various options and windows of the interface, analyzing the final data. Finding problems was not difficult, since they are a part of the students’ routine.

We wanted to understand the sources of these problems, and that is our objective number two. Our research showed that problems such as difficulties getting used to the interface in the beginning of work are essentially due to the complexity of the field this interface is applied for, but other problems can be claimed to stem from an absence of user friendliness and usability. The general approach for solving the tasks and processing the work flow can be improved; thus our last objective is to propose suitable recommendations.

7.2 Proposals

Due to the nature of the field and locations that we have been studying, as well as the limitations imposed on us, we are not ourselves able to develop replacement software. Therefore our specific suggestions for the user interfaces could be said to be educational and reportorial in kind, rather than being intended for actual implementation. Nonetheless we make no possessive claim on them, so they may be used as feedback, input, or reference by anyone willing and able to make use of them, including the manufacturer of the laboratory equipment.

7.2.1 Specific issues

It is our view that most of the issues we have covered in the Research Findings and Discussion chapters could be successfully addressed. Whether the return on investment for such a project would be worthwhile, is a matter for the parties involved to judge; given what we know about the software and hardware used in LC-MS, we think that the issues could be handled exclusively on the software side, since technically they are simply aspects of GUI design and functionality.

A positive note is the slightly unexpected fact that so few of the problems are due to inherent challenges in or limitations of LC-MS; most of them do indeed seem to be isolated to the software. Had they been bound to aspects of the scanning process or hardware, they would likely have been too expensive or impractical to fix, but fortunately this does not seem to be the case. This is a fact that bodes well for the prospects of improving the design.

We believe it would be prudent to improve the communication between the users and the equipment manufacturer or vendor, or make sure that such communication that exists is utilized better.

7.2.2 Future research

Although the problems experienced by the chemistry students do not compromise their work, they do impede it to some extent. It is difficult for us to say what are the wider consequences for this in their area of research, but interdisciplinary studies – particularly how computer science in general and interface usability in particular can and should be applied to other fields – are an interesting topic.
Are there problems of interface usability in this and other scientific fields that are relatively easily solved, yet persist? If so, are there legitimate logistical or economical reasons for this, or is it due to inattention or some other less justifiable reason?

Why isn’t the feedback from users used to improve the software? Are there no channels in place to facilitate this or are they merely not being used? Is this an isolated case or would a wider study show a recurring pattern?

These are questions the answers to which we think would increase the awareness of the challenges and problems with the efficiency of software, and specifically user interface usage in the field of LC-MS (and possibly others as well), which might in time lead to a more deliberate effort to fix them.
Acknowledgements

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The students at SU for allowing themselves to be interviewed, and giving us helpful and detailed descriptions of their work process in the lab.
Ilyar Turdiev for suggesting to us the initial problem.
References


Appendix I: Questionnaire template

1. How do you rate the help you received when you first started working with the software interface?
   [1. Excellent]  [2. Good]  [3. Adequate]  [4. Lacking]  [5. Insufficient]

2. Have you made use of the instruction manual for the interface?
   [1. Yes]  [2. No]

2a. If yes, please select the alternatives that match your experience.
   a) It provided me with useful information that was not available elsewhere
   b) I have used, or do use it as a reference
   c) It did not teach me anything useful
   d) I found it easy to understand
   e) I found it difficult to understand
   f) Other:

2b. If no, please select the alternatives that match your experience.
   a) I found other sources of instruction enough to learn from
   b) Others told me it was not useful
   c) I did not know it was available
   d) I don't like to use physical documentation
   e) I tried to read it but it did not seem like it would help
   f) Other:

3. How well do you think the built-in help documentation in the software covers your needs?

4. What, if anything, do you find lacking about the built-in help?
   a) It can be difficult to find the solution to problems
   b) The solutions to specific problems are sometimes missing
   c) Some explanations are hard to understand or follow
   d) I don't use the built-in help documentation
   e) There's a built-in help? Thanks for the tip!
   f) Other:

5. How do you find navigating your way through the various options and windows of the interface?

6. Is there anything you find lacking about the interface navigation?
   a) It can be hard to remember what some icons/buttons mean
   b) It is not always clear which stage of the process I am currently in
   c) Correcting mistakes is risky - e.g. it may corrupt data or require a restart of the process
   d) Correcting mistakes is time consuming - e.g. it may require redoing more than the faulty step
   e) There is too much dependence on mouse clicks - not enough keyboard hotkeys/shortcuts
   f) Other:

7. How easy do you think it is to go through the data presented in the interface?
   [1. Ideal]  [2. Good]  [3. Fair]  [4. Poor]  [5. Very poor]
8. If necessary, how do you think the presentation of this data could be made clearer?
   a) More customizable tables
   b) Graphical charts
   c) Different configuration of tables
   d) Color coding of features
   e) Interactive features
   f) Other:

9. How much do you value visual representation of data, showing proportions and relations more intuitively but with less precision? Very highly -> 5 4 3 2 1 <- Hardly at all

10. How much do you value numerical representation of data, showing numbers more accurately but with less overview? Very highly -> 5 4 3 2 1 <- Hardly at all
Appendix II: Interview transcript Student A

Val: This is Valentina Rudenok at the chemistry department in Stockholm University, interviewing Student A for our thesis "Interfaces in LCMS", and I want you to tell us about your experience as a student, and how long you've been working here.

A: I've been working here about 1 year on my exam work. I'm a Master's student.
Val: Where did you do your Bachelor's?
A: Not here, but in the environmental chemistry department.
Val: Do you have some background in LCMS?
A: We have been using it in the courses, so yes.
Val: Why did LCMS as a specific part of chemistry, catch your interest?
A: I think it's more fun than GCMS.
Val: What is the most rewarding aspect of the work here?
A: It's the chromatography, the separation methods.
Val: How long have you been working independently with running the tests?
A: I think it's 1 year.
Val: Let's go to the tests that you run and how you deal with the data from those. Can you remember how you felt about this work process when you first started with it?
A: I think it was quite easy because I had a supervisor to show me how to work with the program.
Val: Do you remember approximately how much time it took you to feel comfortable?
A: I think maybe 1 month.
Val: So now you feel quite comfortable and you know how it works?
A: Yes.
Val: What would you say is the best thing about this software, besides the fact that it does its job? Is there something in particular that you like?
A: I don't know if there is a "best thing", it's just software.
Val: Is there something that you don't like, that you would like to be better?
A: I don't like the quantification that the software does, because it doesn't quantify the way I want it to. It quantifies the peaks quite strangely. I prefer to quantify manually, then
Val: In the questionnaire you said that you didn't use the manual. How did you learn?
A: It was my supervisor.
Val: But there were no lectures or specific courses on how to deal with it?
A: No.
Val: So it was personal assistance.
A: Yes, and then I learned on my own.
Val: When it comes to making the presentation of data clearer, you said you want more customizable tables. Can you comment on that?
A: I think it's easier with tables. I want to integrate the peaks on my own and then calculate on my own.
Val: And then about visualization and accurate results. You marked 3 for visualization and 5 for accurate results. Why is the latter more important?
A: I think precision is more important for me than the presentation of the results.
Val: So you are more of a precision person?
A: Yes I think so, and it's important for my results.
Val: When you started out, was it easy to understand what a table means?
A: I think it's easy. It was easy.
Val: So you didn't need any graphs to analyze it?
A: No.
Val: Is there anything we missed or that you want to add about the program? How easy it is to work with it in general.
A: No.
Val: So you think it's a rather good program? You don't have any problems with it?
A: It's just a software, it's not very good and not very bad either.
Val: We want to know if there is something you don't like, what could that be?
A: That would be the quantification part, that it doesn't quantify the way I want it to.
Val: Thank you very much for your information.
Appendix III: Interview transcript Student C

Val: My name is Valentina Rudenok, and I'm at the chemistry department in Stockholm University, interviewing Student C for our thesis "Interfaces in LCMS". Tell us a little bit about your experience here as a student. How long have you been working here?

C: I started my Master's program here 2 years ago. Half of it was lectures, and the other half was practice with LCMS. After 2 years I started with my PhD, which I have been doing for 2 years. So in total, it's 3 years' work with LCMS.

Val: Why did LCMS specifically catch your interest?
C: Because my project major uses the LCMS technique for the quantification.

Val: What is the most rewarding aspect of working here, what do you like the most?
C: It's a very good scientific environment, and we have different people working in different areas like LCMS, GCMS. Some people work with small molecules, others with big molecules, so we have a lot of interaction with each other, a lot of communication.

Val: Let's go to the tests that you run. How did you feel about the work process and the software when you just started. Was it difficult or easy at the start?
C: I cannot say it was easy at the start, because I remember that instrument is not new, it's quite old. The software is a little bit tricky to handle. But as Master's students, when we work with the instruments, we were always accompanied by PhD students, so we could go to them for help.

Val: So you got help mostly for PhD students?
C: Yes.

Val: Was there some course or lecture?
C: Yes, we went through all the serious parts of the instrument on the lectures.

Val: Would you say that you're comfortable with that work flow now?
C: Yes, now I'm quite confident.

Val: Do you remember how long it took from the beginning until you felt "now I can solve everything"?
C: It could be separated into several stages. The first stage is learning to operate the software, not developing the whole technique. Then, after we are familiar with the software, in the second stage we are doing the research independently. Then we go to method development, doing everything ourselves. You really need to know how to develop a method on the instrument, not only how to handle the software.

Val: Did it take a long time getting used to the software?
C: I don't think so, it didn't take a long time for me.

Val: Because of the help you received from the PhD's?
C: Yes.

Val: What would you say is the best thing about this software, besides that it does its job?
C: I mostly use two types of LC instruments, one is an old version and another is quite a new version. The new version is quite a good software. It can handle large amounts of data at the same time and get the results quickly.

Val: Is there something that you don't like about it?
C: There is something I don't like, but it's very specific.

Val: You can say why you don't like that.
C: In each scan, I scan different transitions. Each transition gives me 1 peak. For example, in my scan I have 4 transitions, I should have 4 peaks at the same time. The software separates the 4 peaks into 4 windows. I want them all in a single window, which would make it clear and easy to show in publication. Some instruments do that and then it's very good.

Val: When we asked you in the questionnaire if you find something lacking in the built-in help, you said it can be difficult to find solutions to problems, or that solutions
to specific problems are sometimes missing. Can you tell us a bit more about that, when you search for a specific problem?

C: Most of the time, when I use the help, it's when I'm unclear about a specific concept. For example, what "collision energy" is. I look it up in the software to find the explanation. But when I have some specific problem with an instrument or with a method, I go to the help. It's difficult to find the answer for very specific problems.

Val: You also said of the question if there's anything lacking about interface navigation, that correcting mistakes is risky. Tell me about that.

C: Especially for the old instrument. If you start one run, and realize that you made a mistake such as writing down the wrong injection volume, and want to correct it, then it's difficult to stop that instrument. If you interrupt it, then most of the time you need to restart the computer. It takes a longer time, so most of the time I wait until it's finished and then submit another one.

Val: Does it take a long time to wait until it's finished?

C: It depends on how long you set for each sample, 20-30 minutes. This is not a problem with my new instrument, new software.

Val: You said that to make the presentation of data clearer, you wish for more graphical charts. Is that not good enough in the current software? Why did you choose graphical charts?

C: Normally it just shows you the data in tables, and it seldom has graphical charts.

Val: Why do you think that's important? Would it be easier to understand?

C: Yes, it's easier to compare and have overview for the whole result.

Val: About what's more important, graphical presentation or accurate numbers, can you comment on your answers? You said 4 for graphics -

C: These answers are basically based on the new instrument from Thermo Scientific - it's very good for precision.

Val: We heard from another student that they wanted interactive reports, that the program only gives you tables and that you have to do the rest on your own. Do you think that could be an option, too?

C: Yes, it could be, because actually, for all instruments it's like that - you need to handle data manually most of the time. But for that new LCMS instrument, it can generate data very quickly in table form. It shows even the ration of standard deviation and quantification, you can easily get the result via the software. You don't need to do it by hand.

Val: Is there something you want to add about the software, how you feel about it or something that we didn't ask?

C: It depends on the manufacturing company, how they make the software user friendly or difficult.
Appendix IV: Interview transcript Student E

Val: My name is Valentina and we are here at the Stockholm University chemistry department, interviewing Student E for our thesis “Interfaces in LCMS” and I want you to tell us a little bit about your experience, and how long you’ve been working here.

E: I’ve worked with the MS software here for 1 year, and I’ve had the chance to work with different software – LTQ [linear trap quadrupole], Xcalibur, Sciex, Agilent. I’m a Master of Science student and I’m doing my diploma work here for 1 year.

Val: How much previous experience do you have?
E: At least 4 years as a Bachelor, and for 2 years I did another Master’s in chemistry, so it’s 6 years in chemistry. I worked for a while, not with MS but with other instruments.

Val: Why did you choose LCMS?
E: Recently there has been a dramatic increase in the use of LCMS in research. In the past, GCMS [Editor's note: Gas chromatography-mass spectrometry] was more popular. Now LCMS is more popular.

Val: What do you like the most in this process?
E: The technology, when you have high pressure in a liquid. The interface is so interesting to me, you have a lot of possibility to separate your analytes. The precision of LCMS is much better.

Val: How long have you been working independently with running and analyzing the tests with LCMS?
E: At least 8 months, but I can always ask my supervisor if there is a problem, so I don't think it could be called independent.

Val: When you first started to work with this, how did you feel about the software?
E: My supervisor introduced the software. If there was a problem I could ask her, and I went through the manual.

Val: Was it difficult or easy in the beginning?
E: It wasn't that difficult, the routine work is not difficult but when you're in trouble or you want to restart something from the base, it's difficult so you need some hints.

Val: So you mostly get your tutoring from the supervisor?
E: Yes, exactly.

Val: But there's no specific course or such?
E: No, the supervisor is responsible for helping.

Val: We asked [in the questionnaire] if there was something lacking about the built-in help, and you said "Some explanations are hard to understand or follow", what did you mean by that?
E: Yes, sometimes there are computer science-specific terms that are hard to understand.

Val: You said that you find navigating your way through the different windows in the program "doable", so not really good?
E: There is no shortcut to go from one window to another, sometimes you have to go out completely and then go to another window. It would be good to have the ability to use different windows at the same time.

Val: Then you said that correcting mistakes is risky.
E: Yes, exactly, since for example, if you as per my experience as an analyst want to cancel this sequence, the software gets confused and hangs. Or sometimes if you do data treatment and you want to undo it, you cannot, so you have to close the data and open it again.

Val: Then you also said that, to make the data representation clearer, you want to have more graphical charts.
E: Yes, since it can give you an overall impression of your data.

Val: But there's no graphical representation now?
E: I think it has it, it has a lot of graphical charts but it would be good to have more.
Val: We asked a question as to whether you prefer a more graphical representation or accurate numbers. You said 4 [in a scale from 5 to 1, most to least] for graphics and 2 for numbers.
E: Exactly, since if you can see the overall data, you can make a good decision for the next step. I believe precision is always good for scientific work but for making decisions for the next time, graphical representation is the best.
Val: Is there something that really bothers you with the program, that causes problems?
E: [End of recording, notes say "hard to undo mistakes, there is no error/mistake handling"]
Appendix V: Interview transcript Student F

Val: Hello, my name is Valentina Rudenok, and we are here at the chemistry department in Stockholm University, interviewing Student F for our thesis "Interfaces in LCMS". Can you tell us a little bit about your experience as a student and as a person who works here with this software, and how long you've been dealing with that.
F: I have worked with Xcalibur, specifically, for approximately 3 years. I didn't work very often with that, mostly when I taught a course in mass spectrometry.
Val: How long have you been working independently with it?
F: I only work with it from time to time.
Val: What about LCMS caught your interest as a chemistry student? Why that specific process?
F: I think LCMS is more expansive because of the ESI [electron spray ionization] interface and because I work with proteins, which are more appropriately dealt with through LCMS.
Val: What do you think is the most rewarding aspect of this work?
F: That is a difficult question. There are a lot of advantages of MS. One is that your analyses are more accurate when you run MS because you can have a product ion scan, you can run in MRN and you can choose to run through either the ESI interface, APCI (Atmospheric Pressure Chemical Ionization) interface. So you have different possibilities.
Val: Let's go to the tests that you run and how you deal with the data from those. Do you remember, when you dealt with that software for the first time, was it difficult, or how did you feel about working with that?
F: It was extremely complicated because there are a lot of buttons. It's not really organized from my point of view since I worked with other software, so I could compare. Mostly, what I didn't like was the data processing.
Val: How long did it take for you to feel more or less comfortable with what the program does and how to deal with it?
F: One week of continuous work.
Val: Did you get any help in the beginning or was there a lecture from the manufacturer or your teacher? How did you get to know how to work with it?
F: By myself. Mostly because I had some previous experience with other software, and there is always some logic behind all software. So I used this logic to find the LC, MS, and data processing parts. This is always common for all software, but although it took some time, I managed by myself.
Val: So now you are comfortable with the workflow?
F: Yes, mostly.
Val: What do you think is the best thing about this program, beside that it does its job? Is there something in particular that you like?
F: I have to think. [end of part 1] The easiest thing with this instrument is probably the optimization tuning of compounds, on the tune page. It's quite nice.
Val: Is there something that you don't like about it, that bothers you?
F: What bothers me is that you have to open the instrument from the tune page, then close the tune page; if you don't close the tune page there are communication problems. And also that it's not elastic, it's not organized. You have to go to the instrument setup here, and it should be a bit more organized. It takes a while for a person to understand where they should find things.
Val: Do you think that is a problem of the interface itself?
F: You mean the ESI interface?
Val: No, the software interface.
F: Yes, it's not organized compared to other software.
Val: You said that you didn't use the manual for LC-MS, and that you found other sources of instruction enough to learn from. You said that you taught yourself?
F: Yes, mostly by myself. Other sources that I mentioned -- because I had experience with other instruments -- was my previous experience.

Val: Then you said that solutions to specific problems are sometimes missing in the built-in help? Is that a big problem, can you comment on that?

F: Yes, for example, if you want to find a two-word expression, it will give suggestions just for one word. If you write "add graphics" it will give you a lot of alternatives for either "add" or "graphics" but not for both together. This is the problem: you have to look at all the options to find what you want.

Val: Is that a problem of time, or of effort?

F: It's a lot of unnecessary effort.

Val: You said that you find it problematic to navigate your way through various options and windows. Is that what you mean by the program not being organized?

F: Yes.

Val: About what is lacking in the interface navigation, you said that it can be hard to remember what some icons/buttons mean; correcting mistakes is risky; and there is too much dependence on mouse clicks and not enough shortcuts. Can you explain a little bit about each of those?

F: For example here, I don't know what this (MB) means. There is no explanation of the button, so I have to click to check.

Val: So it could lead to some unexpected results if you click without knowing?

F: Yes, for example the instrument will hang. And here you see there's no explanation at all. I understand that it's labeled but I have no idea what that is.

As for correcting mistakes, if you forgot something. If you put a sequence and you thought "Oh, maybe I shouldn't have done that, because I didn't put the vials inside". If you just press Stop, there is a risk that you have to restart the computer and even the instrument.

Val: "There is too much dependence on mouse clicks".

F: Yes, that's especially true for the data processing. For example, if you want to integrate your peak, there is an integration button but it doesn't show the area, so you have to right click and then go to some options, then find some [end of part 2] kind of other option, then another option in order to get the area. This is the problem.

Val: What about these comments of yours?

F: Yes, the graphics aren't a problem. But I'm not satisfied with online chromatography, when you run e.g. your sequence. Here is the button for online chromatography. Right now it's not running so you don't see anything. When a sample is finished and it goes to the next one, it doesn't show you the previous chromatography. It would be nice if it were to store it. Of course, you can go to the data file and extract it from there. I don't think it would be too much effort to put a button in there to show the previous one. Also, one thing is that when there is too large a peak it doesn't update, so you have to close and open again so that it will update.

Val: So there is no online update?

F: It comes sometimes but it's better to close and open again.

Val: Interchanging between chromatography and spectra are old fashioned, what do you mean by that?

F: This is in the data processing file. If we open, for example, Ramses files. This is a representation of chromatography. This represents spectra. You have to click on that, and then on that one in order for it to work. Sometimes you forget that you want to integrate, and you forget to click on that one, so the integration will not appear. So it's not a necessary thing.

Val: So things that could be automated, should?

F: Yes, it's not necessary to have this kind of activation. You have to make it easier in some way.

Val: When it comes to visualization of data, you said that you don't want any visualization at all?
F: Maybe I didn't understand the question.
Val: The question was mostly about data representation in the user interface: do you want more representation so that it's easier to understand the data, or do you want the program to give more accurate data?
F: The graphical presentation is better for me. I think it manages that.
Val: I'll change your answer, then.
Val: And data precision?
F: You mean the number of decimals?
Val: No, I want to see the balance between the importance, for you, of having better graphical representation or more accurate data in the table.
F: For me, graphical representation is better.
Val: Why?
F: Because I have no need for tables since I work offline with Excel. So for me it's mostly about it showing good chromatography and it being easy to change between e.g. spectra and chromatography. This is the most important.
Val: Is there anything we missed to ask you or do you want to add about this program? Your personal opinion? Any wishes?
F: Wishes? There might be a lot of them. One thing that is very annoying is that when you have chromatography and you want to look at it offline, you have to always press F5 to update it. It won't show you updates otherwise, so you have to keep pressing F5. And I'd like to have more necessary buttons here, like area; not only integration but also show the area. And more organized software. It's confusing sometimes.
Val: Thank you very much.
Appendix VI: Interview transcript Student G

Val: My name is Valentina Rudenok, and I'm at the chemistry department in Stockholm University, interviewing Student G for our thesis "Interfaces in LCMS". Tell us a little bit about your experience here as a student. How long have you been working here?

G: I am master student here in analytical chemistry department for 1,5 year. Next month I am planning to finish my thesis. I just run one LC-MS program, actually there are 2 instruments but the same brand, Thermo Scientific, so I think they have quiet similar program and interfaces.

Val: And how is the program called?

G: Xcalibur. Last year we had like labs only, but not big projects with another program. It was only one run, but I do not remember the name. But for the first impression I find that Thermo is the best.

Val: But why you choose to study for LC-MS?

G: Because LC contains a lot of chemistry, comparing to GC (gas chromatography) comparing to some physical parameters. LC it contains more chemistry, and MS because it is perfect detector.

Val: But was it some personal interest or?

G: ithink this is a future, if I want to search job, it will give me good push. That is why I study for it. So 2 reasons: one is chemistry and another one is a good job opportunities.

Val: What is the most rewarding aspect of working here, what do you like the most?

G: I can not compare so much because I am not Swedish I come from not developed country so it is a big difference in education. But I like the equipment and facilities.

Val: How long have you been working independently with running LCMS tests?

G: From September 2011.

Val: Let's go to the tests that you run. How did you feel about the work process and the software when you just started. Was it difficult or easy at the start?

G: I was with Ulrika, my supervisor, she was sitting next to me and it was easy with her.

Val: But u didn't know anything about it before you started?

G: If you have go good background in analysis you can understand very fast.

Val: Would you say that you're comfortable with that work flow now?

G: Yes

Val: Do you remember how long it took from the beginning until you felt "now I can solve everything"?

G: After 1 week I could solve the problems, I remember that it is a problem in a instrument, I can not solve it because I am not an expert.

Val: What would you say is the best thing about this software, besides that it does its job? What you like about the software besides that it shows the numbers in a table

G: You can easily transform from peak to peak it can make good relation between your parameters, it is very easy.

Val: Is there something that you don't like about it?

G: Xcalibur it doesn't give you automatic report, you have to do it yourself. You have to chose the peak area by your own. I worked before with LCUV, I can’t remember the software but it was giving the automatic report and if you want to make more accurate result you can do it by yourself. Xcalibur doesn’t do it.

Val: So what do you get as a result in Xcalibur?

G: Just peaks, I select peak area by myself, make signal per noise ration, I do everything by myself.

Val: How easy do you think it is to go through the data presented in the interface?

G: It is good but not ideal. I think that there is no automatic report, because I need it.

Val: But will it save your time or it will help you?

G: If I have some mistake in analysis, I can know it from the report.
Val: So it is hard to understand from the peak representation?
G: By the time you will understand, but for the beginner it is hard to understand
Val: Do you think what is most important visualization or data accuracy?
G: Both of them, if I run quantification I want to have accurate numbers to calculate
the concentration in my sample, if I run qualitative analysis I just want to know if this
substance exist or not I think it depends what you do with instrument, but both are
important.
Appendix VII: Interview transcript  Professor A

Val: Here is Valentina in the chemistry department at Stockholm University, interviewing Professor A for the thesis "Interfaces in LCMS". I would like you to tell us a little bit about your experience, what you work with, and how long you've been doing it.

PA: Specifically LCMS? (Val: Yes) Usually I work with Thermo LCMS, both ion trap and triple code.

Val: But you are not a student?

PA: No, but sometimes I work in the lab, though it's not my major task. Since I am a supervisor I have students and diploma workers working with that.

Val: How much experience do you have with LCMS?

PA: Oh, that's a long time. I came here in '97, so let's say 15 years.

Val: So you are very experienced in that area.

PA: And I also teach in mass spectrometry.

Val: How, you think, can you give the best guidance to students who are just starting out with LCMS? What is the most difficult thing for them and how can you help them in the beginning?

PA: It depends on the instrument and how user friendly it is, but I think it's best to sit there and play around. I usually show it to them quickly, maybe only for a couple of hours. That is mainly for Thermo Xcalibur. Then they can play around and learn.

Val: There is no tutorial, lecture, or course on that?

PA: They have to attend the lectures in the MS course. There they also have experiments where they try the instruments, but it's not the same thing to perform experiments in the course. If they have very specific tasks to perform in a course, they don't learn as much as they play around by themselves. But they have to attend the course first, and also the theory.

Val: What do you think is the best way to let them feel comfortable with the program?

PA: The best way is to play around.

Val: In your opinion, how long do you think it takes them to get used to the program and feel comfortable? To be sure that they understand everything?

PA: I would say a couple of days, for Thermo.

Val: Do you remember how long it took for you?

PA: I did it by myself so it probably took a longer time. Maybe one week.

Val: What would you say is the best thing about this software?

PA: It provides a good overview, the graphical design makes it user friendly. You can click on buttons and you'll immediately see what they mean. (Val: Is that for the newest version?) It has always been good, actually, for this instrument, Xcalibur.

Val: Is there anything that bothers you, that you don't like?

PA: It sounds like I'm supported by Thermo now...what is missing there? Actually, I cannot think of anything in particular.

Val: Maybe the built-in help, is it easy to use? (PA: Even the built-in help, they started with very early in Thermo) Is it easy to navigate? (PA: Yes)

Val: When it comes to graphical presentation and accurate data, what do you think is the most important between better graphical presentation - interactive reports - or more accurate data?

PA: Accurate data is by far the most important, even if user friendliness and easy navigation are good. Because we publish our data, accuracy is very important.

Val: How easy is it to correct mistakes if you did something wrong during the workflow?

PA: Easy, I would say, because very often when you make a mistake, it's about you set the things and you have to do the experiment again, so it's not something in the software. It's mostly the analytical workflow, the entire experiment.

Val: Do you have any other comments or some wishes for how it could get better?
PA: What could that be? I can't come up with anything, I'll have to think. I'm sure there should be something. (Val: If there is something that comes to mind, maybe we could note that later) Yes.
Val: Is there anything else you'd like to say to us, about this particular program?
PA: Nothing more other than that I think it's very exciting if you can come up with any ideas to improve it.
Val: Thank you very much.