Factors Influencing the Early Adoption of e-HTPX within Structural Based Drug Design

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Abstract

Innovation is not what innovators do; it is what customers or clients adopt. Put another way, innovation is not brilliant ideas that change minds, but the distribution of useable artifacts that change the lives of the people who use them. To this extent e-Science is moving into a critical stage of its evolution. This paper explores the factors influencing the early adoption of e-HTPX within drug discovery departments of pharmaceutical and biotechnology companies. It considers the techniques used to model diffusion of innovation and looks at how developers could use this analysis improve adoption of their software or services.

1. Introduction

The BBSRC/ DTI-funded e-HTPX project, (an e-Science Resource for High-Throughput Protein Crystallography), aims to produce an easy-to-use resource for protein crystallographic structure determination unifying the procedures for protein structure determination into a single all encompassing interface from which users can: initiate, plan, direct and document their experiment remotely from a desktop machine. See http://www.e-htpx.ac.uk. The protein crystallographic community is made up of both academic and commercial users working in Life Sciences:

- **Academic users;** primarily looking for new protein structures and folds to enhance biologists' understanding of protein function and form;
- **Pharmaceutical and biotechnology users;** need the protein structural data as the basis of structural based drug design.

This paper focus on the factors influencing the adoption of e-HTPX by the protein crystallographers within pharmaceutical and biotechnology companies. The requirements of the academic community are addressed within the project as developers for e-HTPX work closely with users in an academic environment.

2. Demand Side Diffusion of Innovation

Demand side theory of innovation diffusion is based on the cumulative adoption of innovations and technology, typically forming an S-curve distribution. By characterising the potential customers that a product or service is targeted at, these can be broken down further into: innovator, early adopter, early majority, late majority and laggards (figure 1) [1].
These groups have characteristic personality types based on the time of adoption [1]:

- **Innovators** - venturesome, educated, multiple info sources;
- **Early adopters** - social leaders, popular, educated;
- **Early majority** - deliberate, many informal social contacts;
- **Late majority** - sceptical, traditional, resistant to change.
- **Laggards** – the last people to adopt an innovation traditional values, local outlook and resistant to change

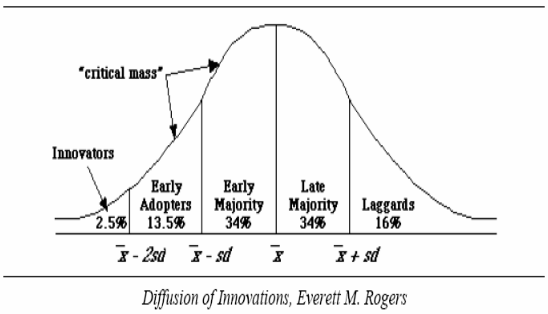

Figure 1: Diffusion of innovation

However the difficulty with implementing this model is that early adopters are difficult to find and require a disproportionate amount of time and effort to locate and persuade. This is compounded by an increasing belief within the IT sector that early adoption of IT gives only short lived competitive advantage [2]. This advantage is outweighed by the disadvantage of paying more for the technology and suffering the majority of the time consuming difficulties encountered during early adoption – the "learning hurdle."

Clearly not all innovations make it to adoption by the majority of members in a social system. There are two recognised stopping points for an innovation before it reaches a critical mass; passing from inventor stage to the early adopters and at the interface between early adopters and early majority. This relates to the different characteristics of the adopter categories and their willingness to work with new technologies and solve difficulties as they encounter them.

Often with new technologies they are introduced with a series of claims and hype from the inventors of the technology, suggesting it will solve a multitudes of problems. For the early adopters of the technology, the innovation may be very attractive and offer enough value for them to risk there time and money in purchasing the product or service. Only when the innovation is put to the test in the real world do the limitations of the innovation become apparent. At this point the potential of the technology reduces in the media and opinions of the early adopter. If the inventors maintain close contact with the new customers of the innovation they can learn from these real life examples and either discontinue the innovation or improve the design giving more functionality and overcoming the difficulties. This process is represented in the Gartner Hype Cycle [3].

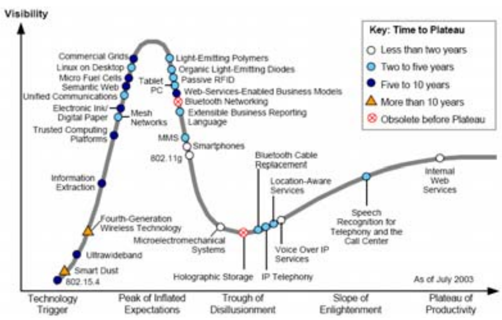

Figure 2: Gartner Hype Cycle [3]

This model (figure 2) suggests the over hyping of technologies at the inventor / early adopter stage to encourage an initial community of users leads to the trough of disillusionment before an understanding of the technology produces an innovation that will attain critical mass and be of value to potential customers. An innovation can be superseded or become obsolete at any time during the hype cycle thus not making it past the inventor / early adopter stage.

For developers of technology these two models are good background information in understanding the position of the innovation Rogers's model (figure 1) gives a good historical perspective on the adoption of innovation and the Gartner Hype cycle is useful at a more detailed analysis of innovations at the inventor / early adopter stage. However these models do not allow us to predict the adoption rates for the product or service for this we need to characterise the technology at a user level.

3. Lesson from Application Service Providers

Application Service Providers (ASPs) emerged in the late 1990's in various guises to offer hosted software applications mainly to small to medium sized business. These organisations offered software applications through a rental type arrangement over a network.

Although there are significant differences between ASP's and Grid computing based web services particularly in the technologies they use to implement the service. They represent the first attempts to move IT infrastructure outside the institutional firewall and because of this have some value for analysis [4].

Over 750 of these ASP firms joined a newly formed industrial consortium between 1999 and 2001, but by the end of 2001 many of these firms had ceased to exist. [5].

Many explanations have been put forward for the demise of ASPs: the failure of ASPs to enhance the customer satisfaction and offer integration [6], the flawed nature of the business model resulting in poor customer adoption [4], an apparent mismatch between the vendor offering and customer requirements [7], and poor methods for evaluating different ASP offerings [8].

When considering software as a service provided over internet protocol an important factor that affects adoption is the relative advantage to the organisation of using a service rather than purchasing the software outright.

Economic advantage of the ASP depends on usage and pricing policy of the service. Relative

advantage of non monetary effects focus on: core competency, scalability, flexibility, risk reduction and faster implementation of programming improvements [9].
The perceived barriers to adoption of software as a service are:

1. Outsourcing risk leading to dependency on a third party or loss of control.
2. Data security; these are an integral part of moving data over public networks [10]. Data confidentiality, access security and general network risks are of primary concern to potential customers [9].
3. Reliability of the service.
4. Other concerns are service stability, longevity and survival of the service. Also recovery of data from an organisation if there is a dispute or the organisation ceases to exist [4].

Currie et al [5] investigating the demise of the ASP's suggested that these organisations had focused on the wrong priorities. ASP vendors tended to emphasise the importance of the attributes such a 24x7 access to remote delivery of software applications; were as the customers were more concerned about security. Also because the ASP viewed the internet as a powerful new distribution channel for existing applications when actually to it required a fundamentally new set of products and technologies [4].

4. Analysis of Potential Comercial Users of e-HTPX

In order to better understand the factors that would determine the how and why scientist within the life science industry would use e-HTPX a series of 21 interview were carried out with potential users.

These interviews described the service offered by e-HTPX, then explored what the potential for this to be used in the protein crystallographer's current working practices. The interviews were recorded using a cognitive mapping process.

Cognitive mapping is a technique to capture the thinking of an individual about a particular issue or problem in a diagrammatic form. The map is designed to focus on the beliefs values and assumptions an individual has about a particular issue [11]. Cognitive maps work well in a messy and complex environment by linking statements made by the interviewee with the context or area of the subject they are related to. By carrying out a series of interviews the Cognitive map can be built to give an overall representation of a community also the subsequent interviewees can be used to validate the opinions of other protein crystallographers.

The aim of the interview was to elucidate the expert opinions of protein crystallographers. The interviews were mostly carried out face to face at the protein crystallographer's organisation.

5. Attributes of Innovations

The precieved attributes of an innovation are one of the most important explanations for the rate of addoption. Most of the variance in the adoption rate of innovation can be explained by five attributes [12]:-

1. Relative advantage
2. Compatibility
3. Complexity
4. Trialability
5. Observability

In addition to these five perceived attributes of an innovation other variables such as; the type of innovation decision; the nature of the communication channels; the nature of the social system in which the innovation is diffusing; the extent of the change agent promotion efforts can play a role in rates of adoption.

5.1 Relative Advantage

Relative advantage is the degree to which an innovation is perceived to be better than the idea that it supersedes. The degree of relative advantage is often expressed in economic profitability or social prestige [12].

So for an e-Science project like e-HTPX, the relative advantage of using e-HTPX rather than physically attending the synchrotron is that there is an economic cost saving in not attending or travelling. However in interviews with potential users of the service it was discovered that this was not a driver for use because the cost of travelling to a synchrotron was insignificant in the total cost of a protein structure solution experiment. This is a clear indication that it is dangerous to make rational assumptions about innovations without testing them against potential or actual users.

The relative advantage of e-HTPX was perceived to be time saving in not having to travel to a synchrotron currently for most commercial users of protein crystallography this means going the ESRF in Grenoble. This may require up to three days out of the Laboratory for the scientist.

Another factor in the relative advantage of using a new innovation is the time that lapse before the beneficial consequences are observed. E-HTPX has an almost immediate return.

5.2 Compatibility

Compatibility is the degree to which an innovation is precieved as consistent with the existing values past expereinces and needs of potential adopters. This compatibility makes the innovation less uncertain to the potential new adopter. Compatibility with previous ideas and tecqniques aid the adoption process.

Increasingly the population are aware of web based service such as banking or share dealing as a service that is provided over internet protocol. By building on this belief system e-HTPX is just seen as another service based software solution.

5.3 Complexity

Complexity is the degree to which an innovation is perceived as relatively difficult to understand and use. When considering the complexity of an innovation it must always be compared with the process that is carried out now.

When considering the ease of use for e-HTPX, it must be placed in the context of a protein crystallographer coming to a synchrotron facility to analysis a protein crystal. Currently they may use numerous different programs to collect and analysis the data as part of their experiment. These software applications available at the synchrotron may be different to the software they are familiar with in their own laboratory.

Balancing the relative complexity of an innovation with the usefulness is explored in the Technology Acceptance Model shown in figure 3 [13]. This suggests the intention to use a technology or software is based on the perceived usefulness of a technology against the perceived ease of use.

The Technology Acceptance Model was developed and successfully used in the 1980's at MIT to investigate the adoption of office based software programs and their acceptance by office workers.

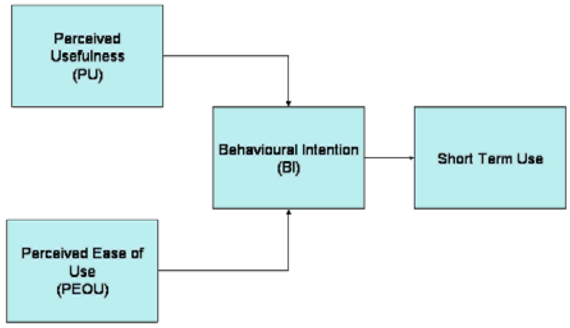

Figure 3: Technology Acceptance Model [13]

5.4 Trialability

Trialability is the degree to which an innovation may be experimented with on a limited basis. The personal trying out of an innovation is one of the ways for an individual to give meaning to an innovation and to find out how it works under one's own conditions.

The trialability of e-science projects is an area that e-HTPX should exploit further this would allow the scientist or potential users to get a feel for the layout and data inputs required to carry out a remote experiment before completing an experiment for real.

Early adopters of an innovation perceive the trialability of an innovation as more important than late adopters [14, 15]. More innovative individuals have no precedent available to follow when they adopt but for later adopters of innovation are surrounded by peers who have adopted the innovation.

5.5 Observability

Observability is the degree to which the results of an innovation are visible to others. For e-Science projects and particular e-HTPX this is a potential problem. Software is already considered as a less observable innovation than computer hardware and because of this has a relatively slower rate of adoption [12]. No longer travelling to a Synchrotron facility may be perceived as doing less work within an organisation and be detrimental to a scientists career, also reduces the opportunities for the protein crystallographers to meet fellow scientists.

6. Drivers and Barriers for the Adoption of e-HTPX

Using a combination of the attributes of the innovation and the Technology Acceptance Model as analysis was then carried out to look for drivers and barriers for the adoption of the e-HTPX service by protein crystallographers within pharmaceutical and biotechnology companies.

6.1 Barriers for Adoption

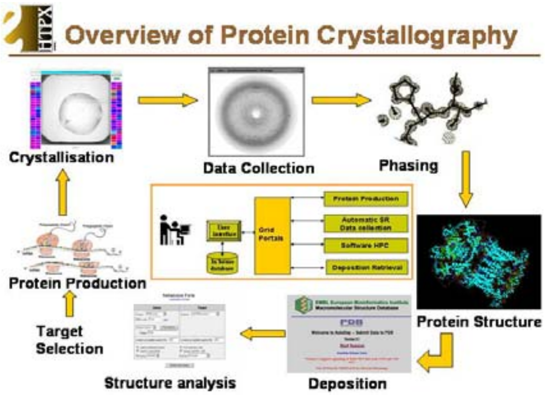

Figure 4: e-HTPX pipeline.

When considering which parts of the e-HTPX pipeline (figure 4) were likely to be used in part of the drug development workflow the interviews revealed that scientist weighs up what can easily be done “in-house” and which processes can’t.

Automation of protein production and crystallisation have become much more affordable in recent years, also grey areas over the intellectual property of the protein production method and ownership of the sample mean that a remote protein production and crystallisation service were currently of little interest within commercial drug development.

Carrying out phasing and protein structure solution requires the scientist to release an amino acid sequence of the target protein that they are working on over public internet which again drew scepticism from the protein crystallographer.

To protein crystallographer within pharmaceutical or biotech companies the main interest is in the remote submission of protein crystals to a synchrotron facility, with the ability to collect screening results and complete experimental data collection on a protein crystal of choice.

The main barrier to the adoption of e-HTPX by protein crystallography was found to be the perceived level of security that was offered by the service.

By limiting the part of the e-HTPX pipeline offered as a commercial service initially to data collection, the project can manage the risk to a user. If some or all of these files were intercepted and decoded there would still be insufficient information to calculate the protein structure or gain competitive intelligent. In order to complete phasing a protein name and amino acid sequence would be required.

By reducing the risk and managing the type of data that is sent over the public internet this does not absolve the project of the requirement for security. In order for the scientists and IT professionals within the organisations to trust the service it must be well implemented. The building of trust in the e-HTPX is extremely important for long term use of the system. If the protein crystallographer intends to use e-HTPX in some situations, this is a moment of truth for the service, if it works well there is a good chance it will be used again.

Trust also relates to the final barrier to use that was identified through the interviews. In order for the e-HTPX pipeline to work remotely there is a high degree of automation that takes decisions on behalf of the user. Control of this automation and the ability to review and overrule the recommendations of the software is imperative if the scientist is to achieve the same results as physically attending the beamline. Protein crystallographers have personal preference within their experimental design, so a scientist will use previous experience and project requirements to alter the experimental parameters. However the automation in e-HTPX will produces one “best” strategy, so it must be reviewed and possibly altered by the user.

Once a user is familiar with the e-HTPX service they may come to trust the automation and use the recommended “best” experimental strategy.

6.2 Drivers for Adoption.

The interviews found that the driver for adoption of e-HTPX was not the cost saving of not attending a synchrotron facility, because when the total cost of an experiment was considered the travel cost were not significant compared with getting the right results.

Ultimately the driver for using e-HTPX would be to reduce the time spent away from the laboratory for the scientist. By using e-HTPX the scientist can progress other laboratory based projects. Related to this, more experienced crystallographers can review and monitor experiments being carried out at a synchrotron, acting as a consultant for other members of their team.

Finally the e-HTPX project is producing XML schemas that define the protein structure determination process by integrating these XML schemas into there own Protein Laboratory Information Systems they can improve the data collection and data mining processes for a Protein Structure Laboratory. This was viewed as having potential in improving the experimental methods used and improving the efficiency of the laboratory.

7. Discussion

Looking at e-HTPX service at a user – features level, this gives the best feedback to the developers of a project. Focusing on the needs of the potential early adopters of the e-HTPX service. These tend to be busy well known protein crystallographers in organisations that use protein crystallography as an important or primary technique in drug discovery.

Like ASP's the difficulties of outsourcing software to outside the organisational firewall is that a loss of control and perceived loss of security of data. This scepticism by the users of the security technologies and there implementation must be overcome in order to attract early adopters to the service, for the commercial sector it is necessary to tailor the e-HTPX service offering primarily a data collection service. By offering the data collection, it is possible to reduce the risk to the organisation, thus removing the main objection and encouraging use.

The modularisation of the service and a focus on data collection increases the importance of the Public Application Program Interface and XML schema, this will allow integration of the results into the organisations own Laboratory Information Management Systems.

This reduction or modularisation of the service to its most useful component from the customer's perspective will encourage adoption. The early adopters that use the service will build trust in the implementation giving two avenues for expansion. Increase the numbers of customers using the service and increase the amount of the amount of the service the customers use.

Modifying Davies, Technology Acceptance Model [13] for distributed software taking into account the findings from the interviews with protein crystallographers about e-HTPX.

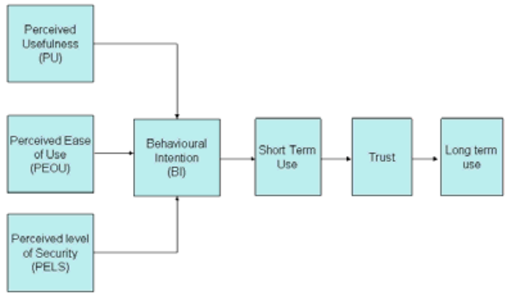

Figure 5: Modified Technology Acceptance Model for distributed software

This model should be applicable to most e-Science projects as a framework for understanding the needs of potential users.

For e-HTPX customer the usefulness of the service is in not having to travel to a synchrotron facility and the returning data in a form that can be integrated with current or new software systems within their enterprise.

The perceived ease of use for a system is a relative statement because it depends on computing competence of the user. Protein crystallography uses lots of different software programs to gain a final result so the average protein crystallographer is quite adept at handling large amounts of data and manipulating it using software. This competence in using software means that ease of use must only be easier than the current situation to be view as an improvement. For e-HTPX service ease of use also means control, it must allow the user to modify experimental conditions as if they were physically present at a synchrotron, this is fundamental to building a user base.

The perceived level of security was added to the model in order to modify the Technology Acceptance Model for networked or distributed software. For the protein crystallographer the security of data was a deal breaker, unless the risk could be managed effectively they would not use the service.

The potential users will weigh up the relative usefulness of the service and its relative advantage to what they are using now. This is balanced against ease of use and the perceived level of security offered by the service. If this assessment is favourable then the potential user has an intension to use the service.

To encourage adoption the service it should be easily trialable. This trailablily is positively related to adoption rate.

Once short term use is established if the project was well implemented and robust, this will build trust in the service. It is important that as well as trusting the service the users see an improvement in work efficiency. This leads to long term use.

From the interviewed protein crystallographers 12 of the 21 (57%) suggested they may use the e-HTPX service under some circumstances, although most of these would only use the service if they (or their IT departments) believed it to be secure.

This behavioural intention to use would have to be converted into actually trying the service described as short term use in the Technology Acceptance Model (figures 3 & 5). Typically there is a large reduction in the uptake at this point, trialabililty of the service is crucial at increasing the conversion rate and encouraging early adopters. For e-HTPX this conversion from behavioural intention to short term use is unknown, this is further work when the first production ready software becomes available.

8. Conclusion.

In order to attract early adopters to e-HTPX from pharmaceutical and biotech organisations it is important to modify the service compare with offering for academic community. Focusing on the data collection part of the e-HTPX pipeline, this step was perceived to have the highest relative value to the scientists and also allows the project to manage the consequence of data loss to the user.

For attracting users to the service a focus on time saving by not travelling to a synchrotron and the ability to integrate the data into existing laboratory information systems will be most productive.

For protein crystallographer the developers should ensure good implementation of security technologies and the ability to override or modify the automation processes to their own preferences.

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