Supporting the Changing Research Practices of Chemists

Research Support Services: Chemistry Project

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Preface

Scholarship, research methods and research practices are in flux as a result of new technology, changing research ambitions and incentives, new data sources and analysis tools, and new dissemination opportunities. Not all fields have been affected in the same way. The changes specific to individual disciplines, fields, or subfields have motivated Ithaka S+R to embark upon a program of research designed to examine changing research methods and practices on a field-specific basis. The projects that constitute this research program are designed to analyze the needs of academics for improved research support services. The recommendations that these projects yield are intended to help service providers—such as libraries and campus IT organizations, publishers, and scholarly societies—to adapt to the changes as they strive to support the work of academics.

As the UK's expert on digital technology for education and research, Jisc has been supporting the work of scholars in a variety of ways for a number of years, including a variety of innovation projects to support the needs of academic chemists. In this project, Jisc supported an in-depth scholar-centric effort to gather essential market research in support of academics and their service providers. It is our hope that these data can be used to design and develop services for which there is essential demand among UK academic chemists. Our goal in this study is to understand at a deep level the evolving needs of the discipline of chemistry and to show service providers how they can modify their practices to meet these new needs. We believe the collaboration between scholars and service providers is essential for the disciplines to develop and thrive.

Following this report's release, we are determined through our partnership to help translate these research findings into implementable services for the academy. One upcoming component of this partnership is a "design workshop" for academic libraries, which will help them to design and ultimately prototype new services that respond to the expressed demands of academic chemists. This new model, if successful, will be an important direction for both of our organizations, in seeking to develop the very best data not for their own sake but in the service of the scholarly enterprise.

Rachel Bruce
Innovation Director, Digital Infrastructure, Jisc

Deanna Marcum
Managing Director, Ithaka S+R

Executive Summary

In 2011-2013, Ithaka S+R conducted an in-depth, scholar-oriented study of the research support needs of academic chemists in the United Kingdom. This report is intended for those who support chemists, including librarians, lab technicians, scholarly societies, publishers, technology providers, and others. The goal of this report is to inform research support professionals about the latest research methods, practices, and information services needs of academics chemists and how they have been changing, inspiring their aims to develop robust, relevant, innovative research support services. While this project focused on academic chemists in the UK, some of the findings and recommendations will be applicable to chemists elsewhere, to other science disciplines, and perhaps even more broadly within the academic community.

The research for this project was based on nearly 60 interviews with research support professionals and academic chemists alike. An advisory board made up of experts from both of these constituencies guided the development of model service concepts, and we subsequently tested these service concepts in a survey of academic chemists.

Based on this research, Ithaka S+R identified three primary thematic areas in which chemists would benefit from new or revamped services:

- We learned that chemists need better support in data management and preservation. Chemists do not have extensive training in how to manage, store, and curate the data that is collected and created by the many members of their research groups. Laboratory groups have a related need for greater support in knowledge management, which includes issues like communication between lab members, transfer of organizational knowledge, and dissemination of information about new research. These research groups are increasingly engaged in interdisciplinary and cross-institutional support, and managing their work effectively requires better technologies, such as enhanced versions of electronic lab notebooks, as well as better data management education and services.
- In information discovery, chemists' interactions with scholarly literature have changed dramatically in the wake of the transition to electronic journals. While highly effective new search tools have developed to help them find information, many researchers remain anxious about keeping up with the newest literature. They need new tools that help them simultaneously stay aware of new research while also enabling serendipitous discovery, which often drives creative new lines of research.
- In the area of research dissemination and scholarly communications, chemists have been slow to place their work in online repositories or adopt new publishing models. Chemists publish frequently, and they require greater support in the dissemination of their many research outputs, including articles, data, and supplementary materials.

For each of these thematic areas, we provide several opportunities for service models through which our recommendations might be realized. These are intended to inspire innovation, design, and prototyping as appropriate within the context of a given service provider.

Finally, in the course of our research we identified three areas of concern for academic chemists that fell outside the scope of this project: laboratory management, gaining access to industrial funding, and teaching support. While we make no recommendations associated with these needs, we would note that some of our in-scope recommendations might be best realized through service models that are broader than the associated needs themselves suggest. Although they are outside the scope of this study, these issues may be helpful in encouraging services providers to think more broadly and creatively about new ways to support scientific scholarship.

Introduction

Across academia, research methods and practices have changed and are continuing to evolve rapidly. Technology allows academics to accelerate many aspects of their research and its dissemination, massive increases in data available for analysis are expanding the nature of collaborative opportunities, and funding models are changing to reshape the incentives for scholarly production. Against this backdrop, it is imperative that researchers have support services available to meet their changing needs. While scholars sometimes have access to new tools to support these changing needs, both entrepreneurs and existing providers require information about the evolving methods and practices of researchers in order to innovate.

The goal of Ithaka S+R's Research Support Services is to bring a scholar-centered approach to gathering information about evolving research support needs. The program aims to provide actionable recommendations for service providers including research libraries, laboratory technicians, campus information technology groups, scholarly societies, publishers, technology companies, and others. Our disciplinary approach allows us to account for the dramatically different needs of individual fields and disciplines. In each discipline, Ithaka S+R hopes to shed light on the kinds of information services that can be provided to support scholarly needs at two different levels: at the campus level, where the projects will identify future roles for the campus library, and at the network-level, where they will identify services that can be provided centrally by scholarly societies or other supra-institutional organizations.

This report is intended primarily for the broad community that supports academic chemists' research. We hope they will suggest opportunities for new services that will ensure that academic chemists and the field of chemistry are well served in years ahead. While our research has focused on the academic chemists in the UK, many of the conclusions in this report will also have resonance in other settings. Our research focused on chemistry as a discipline, and the timeframe did not allow us to examine sub-fields and their practices in great depth.

There were a number of factors that led Ithaka S+R to conduct a Research Support Services project in chemistry. First, like many other science fields, chemistry is not especially reliant on traditional support services providers such as the campus library. The Ithaka S+R Faculty Survey 2009, with a population of US academics, found academics in the discipline of chemistry to be among those who perceived least value in library services other than collections. Second, while other science fields such as astronomy and high-energy physics have moved decisively towards organizing their work on a cross-institutional basis given the expense of gathering data through necessarily shared equipment, chemistry remains to a greater degree campus-based. As is explained in far greater detail in the body of this report, there would therefore appear to be at least a basic logic in considering whether there are support services that an organization like the campus library might be well positioned to provide the field beyond simply collections access. Finally, several notable chemists have expressed concern that the field is not innovating as rapidly as might be hoped. Frustration abounds in some quarters that open access did not take hold more quickly, that informatics-driven research methods have not come into broader use, and that electronic lab notebooks are used only rarely.

The project had several thematic focuses that guided the interviews and helped shape this final report. The interview protocols and the survey were designed to create a holistic view of chemists' research process. Our research focused broadly on the day-to-day workflows of chemists, including how they manage their laboratories, how they collaborate with other academics, and how they interact with their students. We asked chemists to reflect on how they set research goals and how they select new ideas to pursue. We also gave close attention to their research process, with investigation into how they conduct desk research, use online research resources, gather data, and keep notes. Finally, we focused on how chemists fund their research and publish and share their various research outputs.

Ithaka S+R found that UK academics in chemistry face growing pressures. They must manage their labs more efficiently, secure funding more creatively, maximize the impact of their research outputs, and maintain current awareness of the burgeoning publications in the field. Chemists need services to make their lives easier and their research groups more productive and impactful. Few of the services they need fit directly within the traditional scope of any type of provider. This report lays out these issues in greater detail and describes a series of recommendations that draw on our research findings. Each of the recommended services will require substantial design and innovation from any provider that may choose to try to address them.

Methodology

The project was made up of three research phases. The goal of this phased methodology was to approach iteratively the challenges facing chemists and the professionals who support them. Phases I and II were made up of qualitative interviews with research support professionals and chemists, respectively, while the final phase consisted of a survey of UK academic chemists.

The project was guided by a six-member advisory board of academics and others with a close knowledge of academic support services for chemistry. A list of advisory board members is available in the Acknowledgements section of this report. The advisory board helped shape the project's scope, the list of interview candidates, the thematic focus of the interview guides, the survey questionnaire, and our findings and recommendations.

For Phase I of the Research Support Services for Scholars Chemistry Project, Ithaka S+R interviewed twenty-three research support professionals from a variety of organizations and higher education institutions in the UK. Nine of these professionals were science or chemistry librarians. The remaining fourteen were from other campus entities outside of the library, or from external organizations. Interviews were primarily conducted via phone conversations; each interview was about 60 minutes in length. Interviews were recorded for transcription and analysis purposes. Interview questions focused on three areas: current services provided to chemists, planning for future services, and challenges. All of the interviews were recorded with the permission of the interviewees.

In Phase II, Ithaka S+R conducted one-hour interviews with 33 academic chemists in the UK These chemists were chosen for the diversity of their research topics, as well as the diversity of their institution types and department sizes.

In order to encourage candor in the interviews, we have kept all researchers' comments anonymous. The majority of the interviews were conducted face-to-face, but others were done over the telephone. The interviews followed the same format as those in Phase I.

Interview protocols for Phases I and II are provided in Appendix A, while a full list of all interview subjects is provided in Appendix B. To protect confidentiality regarding candid institution-specific interviews, it is not possible to release recordings or transcripts of these conversations.

In Phase III of the project, Ithaka S+R conducted a national survey of UK academic chemists, with the assistance of the Royal Society of Chemistry (RSC). This was a non-scientific survey that was intended to confirm some of the preliminary findings of the interview phases, as well as to test several new service concepts for chemists in the UK. RSC emailed an invitation to participate in the online survey to an opt-in list of 6,356 of its member chemists in October 2012. This list included professors, readers, senior lecturers, lecturers, graduate students, and postdoctoral researchers. The survey was open to responses for two weeks. There were a total of 149 completed responses to the survey, for a response rate of 2% percent. We will use the data from the survey to illustrate some of the themes throughout the paper. However, the results should not be construed as being representative of the opinions of chemists in the UK.

In this report, we refer regularly to universities, libraries, and chemists. Unless otherwise specified, these references are specific to UK universities, UK academic libraries, and UK academic chemists.

Acknowledgements

A number of individuals contributed to this project, and we express our gratitude. We thank first of all Jennifer Rutner, the senior analyst who during her time at Ithaka S+R conducted nearly all of the interviews that constitute a significant share of the research on this project. In addition, we thank the members of this project's advisory board, who helped formulate the scope and coverage of the project, assisted in identifying interview candidates, and reviewed the analysis and recommendations that appear in this final report. Our advisory board members are:

- Neil Berry, Lecturer in Chemistry, University of Liverpool
- Frances Boyle, Associate Director, Library Academic Services, Imperial College London
- Simon Coles, Director, EPSRC National Crystallography Service, University of Southampton
- Richard Kidd, Business Development Manager, Strategic Innovation Group, Royal Society of Chemistry
- Cameron Neylon, Advocacy Director, Public Library of Science (formerly Senior Scientist, Science and Technology Facilities Council)
- Ben Showers, Programme Manager, Digital Infrastructure, Jisc

In this project, Ithaka S+R researchers interviewed both chemists and research support service professionals, each of whom gave generously of his or her time to ensure that as balanced as possible a perspective could be presented in our analysis. They are listed by name in Appendix A, and to each of them we offer our deepest thanks.

The development of this project, its analysis, and the final report were reviewed formally and informally by every member of the Ithaka S+R team. We offer special thanks to Kevin Guthrie, Nancy Maron, Deanna Marcum, and Kate Wulfson, for their comments on various drafts, and to Heidi McGregor and Jeremy Stynes for assistance with production, design, and communications. We also thank Leah Rae McEwen of Cornell University for her constructive feedback.

Finally, this project could not have been conducted without the funding made available through Jisc. Rachel Bruce was an early champion of the scholar-centric approach this project has taken, and Ben Showers has served to guide the project's development not only as a key member of our advisory board but also in developing mechanisms to maximize the impact of our analysis and recommendations.

While the work of this project was aided by the enthusiasm and support of many individuals, we take sole responsibility for the contents of this report.

Findings

This section gives a summary of the project's high-level findings. Each heading corresponds to a more detailed section in the body of the paper that describes the results of the research project in greater detail.

Research Teams and Collaboration

- Most of chemists' research work is conducted collaboratively at the level of the lab group. The members of the group work on one large research project or on interrelated projects, rather than as "lone scholars," and consequently their research support needs are best understood collectively.
- Academics who lead laboratories guide the direction of their research group, but their work is largely devoted to management activities. They must oversee all of the work of the lab, obtain funding for students and for specific projects, publish research findings, and participate in the activities of their department or institution. Since they are infrequently involved in day-to-day research tasks, they are not always the lab members most in need of direct research support.
- Undergraduate and graduate students receive apprenticeship-like training within the context of their research team. Advisors actively manage their students. The relationships between postdoctoral researchers, graduate students, and undergraduate students also provide important opportunities for mentorship and training.
- The work of the traditional lab group is increasingly complicated by multi-disciplinary, multi-institutional collaborative projects. Chemists work with research partners in other departments and at other institutions, and their graduate students work in multiple labs under different advisors. Research support professionals face new challenges in supporting this collaboration.

Library Use and Research Resources

- Chemists value academic libraries primarily for the access that they provide to electronic journals and other online resources. The relationships between campus libraries and the departments remain focused on collections budgets and the acquisition, provision, and maintenance of journal subscriptions.
- Beyond their collections, most libraries provide few services that are highly valued by chemists. Most institutions have closed their departmental libraries and consolidated services into a science library or the central library. Many existing services are focused on students' needs rather than research support. In many cases, libraries are limited in the amount of staff time and financial resources that they can devote to new service models.
- Many of the important research resources that chemists use are from providers outside of their institution. Chemists expressed satisfaction with many of the research tools that are available to them from technology companies, publishers, scholarly societies, and other sources. These groups are responsible for much of the ongoing innovation in research tools for chemists.

Tools for Discovery

- The creation of electronic journals and their widespread availability compared with earlier approaches to dissemination has brought about broad changes in the ways that chemists interact with the scholarly literature. Chemists, who have always needed to keep up with the latest research, now feel more pressure to do so as the amount of online content that they have available to them continues to grow.

- Instead of flipping through journals to maintain current awareness, chemists' interaction with the scholarly literature is now primarily driven by keyword and other searches. Chemists are very satisfied with the available tools that allow them to search for articles, data, and other information, but they lack resources for maintaining awareness of the newest scholarship directly relevant to their interests, or for serendipitously discovering scholarship not previously understood to be related to their needs. New research technologies have generally focused on the search-driven mode of content discovery.

- Review articles, conferences, and informal discussions with colleagues remain important parts of the way that chemists learn about new research outside of their area of expertise. These sources remain the best mechanisms for serendipitous discovery, and they also provide chemists with a condensed format for maintaining awareness of new research.

Literature and Research Notes Management

- Electronic lab notebooks, or ELNs, remain unattractive to most chemists as an option for knowledge management in the laboratory setting. This is in part because the hardware is not suited to all lab environments, but it is also because the available systems do not provide enough convenience and utility for users.

Managing and Sharing Data

- There is widespread misunderstanding among chemists about what constitutes effective data management practices. Data are often stored in impermanent formats that are at risk of technological obsolescence. Labs give little attention to creating proper metadata for their research data, and important knowledge is lost over time as graduate students and other junior researchers leave the group.

- Most universities are still in the early stages of developing support services to help scholars deal with data management. This responsibility is being taken on by different departments and functional units at each institution.

- Many chemists are resistant to the idea of openly sharing their data. However, while open sharing of data is not the norm in chemistry, researchers frequently disseminate their data informally when it is requested by colleagues. There is also a sizable minority that uses online repositories for sharing some of their data.

Research Dissemination

- Chemists reporteded publishing an average of 3-6 original research articles per year. Chemists publish in relatively traditional article formats, and they place a strong premium on publishing in the best regarded journal that will accept their work. Chemistry articles are usually accompanied by supplementary data, and the data that they present become the building blocks of research and reference databases assembled by publishers and other providers.

- Chemists do not have a strong preference for publishing in open access journals. Many chemists are very satisfied with the access that they have to scholarly literature, and they question the need for highly technical scientific publications to be broadly accessible by the public. Some researchers are also biased against open access journals because of what they perceive to be those publications' lower impact factors.

- Posting copies of pre-prints or published articles in institutional repositories or subject-based repositories has not caught on widely in chemistry, though in some cases chemists have deposited their research outputs as part of the Research Excellence Framework evaluation process.

Funding

- The changing directions of public funding in the UK have had substantial impacts on the shape of research. Most chemists reported that the availability of funding has significant impacts on the subject areas that they pursue, and they have perceived a marked increase in the difficulty of obtaining funding from the EPSRC (Engineering and Physical Sciences Research Council) and other sources of public funding.
- Due to pressure from funders, lack of available funding, and natural common interests, chemists have strong interest in working on projects in collaboration with industrial partners.
- University research offices have become important service providers because of their role in ensuring the success of industry partnerships. They are also highly valued by many researchers for the role they play in easing the burden of applying for public funding.

Research Teams and Collaboration

Chemists functions in lab groups, rather than as individual researchers, and our survey respondents reported an average lab size of 12 individuals. They conduct complex research projects that require the time and resources of many chemists, students, and technicians, and they work in collaboration with other scientists at their own institutions and in other countries. Group-based work is the standard, with a faculty member leading and supervising a team of students. Groups can range from three to a dozen or more students at all levels of study, depending on the scope of the projects and funding the faculty member has secured. Students go through an intensive training period where they effectively serve as apprentices and develop a gradually increasing level of independence. Senior researchers can devote only a small percentage of their time to research because as leaders of a small research enterprise, they have many administrative tasks that they must accomplish.

The Role of the Lab Leader

Chemists in academic positions usually lead a group of researchers that vary in size depending on their research topics and funding sources. The group functions as a single unit when it designs and performs research. There are three different parts of research: formulating the project, performing the experiment, and interpreting what the results mean, and each of them can be completed by different people within the lab group. The lab leader generates new ideas and seeks the funding to carry them out. But in addition to these roles, the lab leader must deal with many of the administrative and planning tasks, such as recruiting new graduate students, finding collaborators, monitoring the ongoing progress of the project, and performing all of their teaching and other institutional responsibilities. Many senior scholars take on so many diverse roles that they feel pressure to spend most of their time in areas other than research. Some researchers expressed weariness over their administrative duties, which keep them away from what they see as their primary role in the lab. As one scholar put it: “I enjoy doing research. I enjoy doing teaching. I do not enjoy paperwork. I would like to be able to spend more time in research rather than administration.”

Finding support for graduate students is one of the most important tasks of a lab leader. Student positions are typically funded directly from grants, though some departments do have a budget to support PhD positions. The EPSRC program on Centres for Doctoral Training (CDT) has made substantial shifts in the way that chemists fund their students; it has concentrated students around thematic research areas at particular universities. As part of the program, institutions take a more systematic approach to training their PhD students.. For example, at the University of Bath Doctoral Training Centre in Sustainable Chemical Technologies, each PhD student is assigned two advisors–one academic and one from industry–to shape and guide the student’s research.[1] The CDT model sometimes incorporates an extra year of training into the graduate program and focuses on developing a group of students as a cohort. The long-term impact of the Centres for Doctoral Training has yet to be seen, but many chemists reported frustration with the increasing difficulty of obtaining funding for single students or small groups of students. Some researchers, especially those in small departments that cannot support a CDT and those whose research does not fit the thematic focus of their institution, feel that they have no means of funding new PhD students.

Students in the Lab

Chemists vary in how much responsibility and independence they give to their students, both at the graduate and undergraduate level. Most chemists prefer independent students, and interviewees said they tend to spend the most time with the students who are lagging behind. Unlike in the humanities, where faculty members advise students on their own independent research, faculty members in chemistry act as managers who oversee their students’ work in collaborative projects. Much of the day-to-day management of projects, as well as the actual experimentation, is left to the graduate students and postdoctoral researchers: “They’re working in the lab. They have to make decisions in terms of the things that they’re doing. I don’t speak to everybody who’s working on it every day, but I speak to them regularly, and we have regular meetings to go through the progress that they’ve made.” One professor said, “The way I like to do things is define a project and then basically let the students run it.” In other labs, all of the students work on discrete tasks that are part of one large project, which requires more coordination on the part of the lab leader. Some chemists like to follow their students’ progress more closely by checking their lab notebooks daily or weekly. If nothing else, the lab leader is the undisputed financial manager of the group: “In terms of the actual work and sort of sourcing materials and equipment and things, they arrange that all themselves, and then they just bring things to me when they need…signing or approving or orders placing.”

1 University of Bath Doctoral Training Centre website: http://www.bath.ac.uk/csct/dtc/

Projects are generally defined by the funding that is available, and this in turn defines the career of a PhD student because it determines what they will be doing in their research.

While the relationships between PhD students and lab group leaders can sometimes be very informal, several professors said that they have regularly scheduled review meeting with the students to talk about their performance and their progress toward a degree. Chemists frequently share graduate students with other professors, sometimes across department lines and other times across institutional lines. These arrangements are generally dictated by funding. Students may have two advisors, or work in two separate labs on different aspects of their research. Some graduate students find it difficult to navigate the challenges in coordination and collaboration that arise from their interdisciplinary work. In addition to their relationships with their advisor, graduate students must develop relationships with the other members of their lab. In many labs, experiments run 24 hours a day and students work in organized shifts. They must trust each other to perform certain tasks on their behalf when they are not present.

Undergraduates can do some of the same basic lab work as graduate students, but at a lower level than graduate students. In some research groups, graduate students and postdoctoral researchers take on responsibility for overseeing their work. This apprenticeship helps them learn the skills that they may need if they continue their studies. Undergraduate students in chemistry are much more likely to stay at the same institution for their graduate study than they are in the United States. At some institutions, undergraduates can apply for small grants from their institution to fund their research. One interviewee mentioned that he encourages his students to seek funding from the Nuffield Foundation, which supports undergraduate STEM research. Professors generally guide their students by helping them develop independent projects that will feed into the work of the lab.

Collaboration with Other Researchers

Chemists collaborate frequently with other chemists or scientists working in related fields. These working relationships often span universities and involve labs from multiple countries. Frequently, collaborators are brought in because the research team needs to fill a gap in their expertise. Sometimes a collaborator can help with relatively simple needs that are not at the core of the project, such as synthesis of a needed molecule, but other times they provide higher-level consultation and analysis. For example, one researcher said that he has worked with a theoretical physicist, who helped him interpret results that he could not otherwise explain. Other collaborations are marriages of convenience, where one side has equipment or expertise that will fit nicely into the overall goals of the lead researcher. Sometimes these working relationships can last for a long time. As one researcher observed:"There are quite a few of the [established collaborations] and I think because they are established in terms of producing results in papers, then each side knows what the other side wants." The researcher who is leading the project gets access to more resources than he or she would otherwise have, and the secondary researcher gets a "free" publication in exchange for very little work.

Researchers have different means of identifying potential collaborators. Sometimes they look for other scientists at their own institution, sometimes they meet them at conferences, and other times they contact people whose articles they have read. Several chemists said that Web of Science and SciFinder can be valuable in helping them identify collaborators; they use them to explore the current areas of interest of their colleagues at other institutions. (Some chemists also use it as a way to track labs that they view as competitors who are working in their research area.)

Chemists maintain a great deal of independence within their collaborative relationships, and communication can sometimes be the biggest barrier to producing successful work. In many collaborative arrangements, each side performs its experimentation and analysis largely independently of the other. This is especially true in interdisciplinary collaboration. One chemist who works with a group of biochemists said that email is a sufficient means of communication because his research partners do not have the expertise to review his data, so they do not need to transfer the files. Collaborators often share data over email, unless files are too large. Researchers are often frustrated by an inability to get all of the data that he or she would like from a collaborator. One chemist said he goes as far as to avoid crystallography services at other institutions because he always trusts his own data more. One interviewee said she has a grant to collaborate with a lab in a developing country, which poses significant challenges because her colleagues there have a poor internet connection. Instead, they rely on visits to her lab in the UK, where they can use the library resources and focus intensively on their project. When they return to their home lab, they can continue the experimentation and prepare for the next research trip.

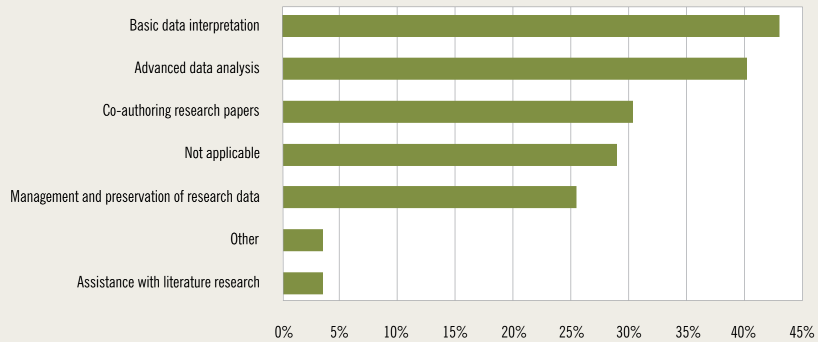
Truly innovative collaborative projects and relationships that last long beyond the period of the grant are rare. One senior researcher said that interdisciplinary collaboration often happens in areas where neither side (or only one side) is doing work that is groundbreaking in their field: "Constructing collaborations where you have people who have genuinely different disciplinary expertise, and each of them are working effectively at the top of their game, that's actually quite challenging and is very often just not possible." Sometimes chemists develop long-lasting collaborative relationships that last well beyond the term of a single project. One chemist told us that his work with another chemistry professor at his institution had gone on for about a decade; their proximity makes it easy for them to talk on a daily basis.

Collaboration with Lab Technicians

In addition to their fellow researchers, chemists often work with a range of other lab support personnel. Most institutions with large chemistry departments employ technicians to provide help with shared experimentation equipment. Many of these service providers who run x-ray diffraction, crystallography, and NMR spectroscopy labs are themselves chemists with doctoral-level degrees and independent research interests. Every institution has its own way of managing and staffing shared equipment. We observed several models for managing these services. At some institutions, a faculty member serves as the "academic manager" of the service, while a technician runs its day-to-day operations. This multilevel management of shared labs occurs at many institutions. In some departments, only the technician is allowed to operate the equipment, while in others, anyone who has been properly trained is allowed to do so. One lab manager told us that it would be helpful to have a better booking system for the equipment so that this process could be less manual.

FIGURE 1

If there is a lab technician or other staff member who manages specialized research equipment at your institution (i.e. equipment for x-ray crystallography, NMR spectroscopy, etc.), do they assist you with any of the following?



While some of these research support professionals do nothing more than operate lab equipment, others are much more closely engaged with the academics who they work with. In the survey, a significant percentage of respondents reported that lab technicians at their institutions have helped them with advanced data analysis, data management and preservation, and have appeared as co-authors of their published papers (see Figure 1). These institution-specific roles are among the most important collaborative support providers for chemists.

Library Use and Research Resources

Chemists are heavy users of their libraries' collections of electronic journals, and in most cases are satisfied by the collections that are available to them through the library. However most academic libraries do not offer campus-based services that chemists perceive as being of high value. Many of the most important research resources that chemists use are provided by publishers, technology companies, and other organizations. Sometimes these are licensed by their institutions, but in other cases they are available to researchers directly. This report will not attempt to list these services comprehensively, but will instead some of the issues related to their use by academics.

Campus Libraries

Most chemists value their library primarily for its collections. Few chemists visit the physical library with any frequency for their own research, but they are highly active users of the digital collections that libraries provide. Most of our interviewees were keenly aware of the role their libraries play in purchasing and curating the materials that they have access to, and many campus libraries work closely with their chemistry departments when they make collections management decisions. On the other hand, few chemists said that they value any of the services provided by their central campus library. Some researchers know the subject specialist who is assigned to their department and work with them occasionally, but none of our interviewees had developed a close working relationship with a librarian.

Library Services

Interactions between librarians and chemists are relatively rare, and when they do occur, they are most often focused on collections. In the survey, fewer than 10% of respondents reported that they had either had a research consultation with a librarian, asked for help with a data management plan, or asked for assistance on an issue related to publishing in the past year. By comparison, 53% said they had ordered a book through inter-library loan in the same period. Collections-related services like ILL remain the most important library services to academic chemists.

Perceptions of the library's role remain rooted in traditional services. Some chemistry librarians noted that while their libraries are considering new roles and are interested in data management, open access, copyright, grant writing, institutional repositories, and open notebook science, chemists do not typically reach out to the library to discuss these issues or request support. One librarian interviewee recognized, "We can be slow to embrace new things," in reference to implementing support services for new technologies. In another case, when discussing a campus-wide data management strategy, a librarian stated that the library is interested and involved, but not taking the lead in defining what the library's role could and should be in this initiative. In recent years, some libraries have been forced to scale back plans for new services because of budget cutbacks.

As the ease of electronic access has grown and budgets have been constrained, most chemistry departments have eliminated their departmental libraries. There is no longer a need for chemists to be physically close to collections of print journals. At the institution where one of our interviewees is based, the departmental library was recently dismantled and the space was converted into a common room and computer lab for students. The books were sent to the main library. However, there may still be a role for departmental libraries, if they have the right combination of physical convenience, ample funding, and knowledgeable staff. The departmental library at Cambridge University was pointed to as a model of excellence by current and former students and researchers. Faculty who said they would normally never visit the library said that at Cambridge they would stop there to use the library space for study and consult the librarians about research questions. The library also offers research training for students who are new to chemistry research and need an introduction to the databases and tools available to them.

Most libraries have continued to use a departmental liaison model to serve faculty members in chemistry, but in most cases this model has not produced deep collaboration between faculty members and librarians. At universities with large chemistry departments, the liaison role still exists, and subject specialist librarians can serve on academic and departmental committees, attend faculty meetings, and maintain regular contact with the chemistry department's faculty liaison to the library. At many institutions, however, one librarian is responsible for multiple science departments, which leaves them little room to specialize or provide detailed research guidance to researchers. Many librarian interviewees remarked on the increasing distance, both physically and intellectually, between libraries and chemists. Chemists' meetings with librarians tend to be few and far between, when they do occur they tend to be focused on collections. Many chemistry and science librarians may not bring to their positions the types of expertise they would need to engage more deeply on chemists' research projects. Several chemists said that in an ideal world, they would find it more useful to have someone who could work with their lab on a regular basis and thus develop a better understanding of their research needs. "They can provide you with sort of general guidance and can tell you what facilities are available, but you effectively have to do the work yourself." Research support professionals in other sectors supporting chemistry tend to be staffed, to some degree, by trained chemists, including PhDs and practicing researchers. For the most part, libraries have not attempted to reproduce this model.[2]

While the demand for library services appears to be relatively low, there are hints of demand for new services in certain areas, especially in the area of publishing. Some researchers are looking to the library for leadership and advice on issues of copyright and open access policy. At one interviewee's institution, the departmental representative to the library invited the institution's repository manager to come and speak to the department about the repository and its role in preservation and access. Another researcher said that he expects that the library will take charge of implementing any new open access mandates from RCUK: "I suspect that they will be the people that will be put in charge of…making publicly funded research available." This emerging demand from researchers may continue to grow as the debate on open access in the UK continues.

Library Collections

Collections remain central to the research support that academic libraries provide to chemistry departments. Online journals and databases are very important to chemists' work, and many researchers expressed satisfaction with the resources that their libraries are able to purchase for them. Most chemists use almost all library materials online, though in some cases they must still visit the library to use a resource. With cuts to chemistry collections budgets at many institutions, librarians have reached out to faculty to get their expertise on how to effectively and sustainably curtail journal subscriptions. Both librarians and chemists mentioned that the consultation over journal subscriptions has helped improve collections development and management, and it has also made scholars more and more aware of the budgetary limitations facing their libraries.

The most frequent point of contact between chemists and librarians is when either group reaches out to the other to engage in discussions about collections. This can happen on a frequent, informal basis, when a subject librarian emails members of the department to ask about their journal needs, or when a researcher makes an inquiry about a particular journal. Many libraries have a separate budget for chemistry acquisitions that they use for journals, books, and ILL requests. If a faculty member makes a request, the purchase will come out of this fund. As is the case with library budgets more generally, these chemistry acquisition budgets have been cut back in recent years, forcing librarians to think carefully about how to manage subscriptions. Generally, they will contact the department before they make cuts, so that they can make them in a targeted way that will mitigate the impact on the department. At one institution, the librarian who is responsible for the library's chemistry acquisitions budget attends the

2 For more about hiring subject matter experts with experience in the sciences, see Donna M. Beck MLIS & Rachel Callison MLS (2006): Becoming a Science Librarian, Science & Technology Libraries, 27:1-2, 71-98

department's faculty meetings to gather input about collections. This librarian also brought members of the department to meetings with a representative from a major database provider. Librarians frequently seek feedback from chemists about their collections priorities, and in many cases they ask them to trial a subscription or tool in order to evaluate it before purchase. Some smaller institutions struggle with inadequate access to journal literature, but few chemists said that it inhibits their research, and many said that they had seen improvements over the past decade. For example, one professor remembers when his institution had a single-user license to SciFinder, and said that it is now comparatively easy to get access to what he needs.

No matter how they get access, most chemists feel they can get all of the materials they need. When they run into material that they do not have access to through their local library, there are a number of strategies that they use to get access to content. The first option for many chemists is to make a request for an inter-library loan or to get an article through the British Library. The British Library's document supply services are a comprehensive last resort option for materials that researchers cannot access anywhere else. Many chemists use this service, though several complained about the time limits and printing limitations that come along with PDFs delivered this way. Another option is to visit another library. For chemists in the London area, one of the best options for accessing materials that they would otherwise not have is to go to the British Library themselves or to send a student there on a research trip. Another interviewee mentioned that he had used the RSC's library to get access to materials that he did not have through his library. A professor can also make a request that his or her library purchase the material. Only one chemist who we spoke to mentioned that he had requested that his library buy particular books in the past, but he said he had been very pleased with this service and he had received the materials quickly. Many chemists will simply email the author if they cannot get a copy of a journal article. "It happens to me quite often as well, that people cannot access my papers and they ask me whether I could send them a PDF file, and I don't have any problem with it. I don't know whether I'm violating and copyright issues with it." If this doesn't work, they will email a friend at another institution that does have access. It is difficult to quantify the effect that this informal sharing has on access to the literature.

Teaching

While support for students and information literacy instruction was outside the scope of this project, it is an area of strong interest for librarians, and it is one area where some chemists perceive need for library services. Relatively few chemists invite librarians into their classrooms to give presentations to their students about the research process; in the words of one librarian, "It's no longer necessary for me to train them on how to use databases." However, librarians said they continue to work with students outside the classroom to introduce them to their libraries' digital resources, demonstrate tools for citations management, and introduce them to more advanced searching techniques.

Many chemists have come to see the library's services as primarily student-facing, and they value the library for their role as a resource for teaching. Many chemists said that they last time they visited the library was when they looked at books that they are considering assigning to their students. Moreover, several interviewees mentioned that the creation of more undergraduate study space was a priority for their campus library. While few faculty members said they would be likely to use library space for research, they have observed that their students have benefited substantially from having this additional resource available. One professor said, "The university library…has a big refurb on the ground floor, and the support services that go with the library are absolutely excellent. I just don't need to use them because, quite rightly, they're student-oriented."

Chemical Information Resources

This project was not intended to gather information about specific online journals, publisher platforms, databases, or information management tools. However, the interviews revealed a number of important trends in how these resources are created and used, as well as how they relate to campus-based services. Publishers, technology providers, scholarly societies, and other entities have created a variety of tools to serve the information needs of chemists. With libraries playing a smaller role, these tools are now the major source of innovation in how chemists locate data, literature, and other information.

Chemists are relatively happy with the tools they have available to them now for searching for chemical information; 59% of survey respondents agreed with the statement, "The tools that I have for searching for information about chemicals are sufficient to my needs." They are even more satisfied with their abilities to search for literature; 68% agreed with the statement, "I have access to excellent tools for searching for scholarly literature." Many interviewees reported having experimented with new tools and platforms. These new services are driven by demand on the part of researchers or available funding from grant making organizations, and their success or failure depends on the uptake of their products.

There is continued innovation among the information services products available to chemists, and this report will not attempt to catalogue the various new products that are being made available by providers in the UK and around the world. Two UK-based examples of how to create and provision chemical information are the ChemSpider and Dial-a-molecule. ChemSpider, now a product of the Royal Society for Chemistry, is an open database of chemical structures from hundreds of published sources, and invites contributions from the chemistry community.[3] Dial-a-molecule is a an EPSRC Grand Challenge Network that aims to enable "100% efficient synthesis" of molecules through a network of experimental data. Additionally, The RSC will soon be taking over the Chemical Database Service, which has helped centralize chemistry data collection and provision in the UK. The new National Chemical Database Service may provide new types of opportunities for researchers to share and reuse data.[4] Each of these initiatives is taking a critically important broad view of supporting chemistry research in the UK and abroad through data management.

Many of the newest efforts to create new tools and services have included attempts to break down traditional barriers between proprietary information systems. In chemistry, as in other disciplines, there are many information

3 ChemSpider website: http://www.chemspider.com/

4 CDS website: http://cds.rsc.org/

"silos" for chemists to access in their research routines, each with individual infrastructures, organizations, and search tools. Many research support services are focused on bringing these resources together, improving searchability, and greatly increasing easy access to information for chemists.

Many of the support services that already exist suffer to some degree because they do not have effective tools for outreach among faculty. Librarians are not close enough to the faculty to fill this role, even for products to which their library subscribes. This creates a gap between the products available, which often fill a very specific niche, and the scholars that they are meant to serve. For example, many chemists complained that they do not have an effective way to manage their own personal collections of journal articles on their computer. In many cases they were unaware of the variety of tools (such as Mendeley) that are already available for this purpose. Librarians at most institutions have not taken on the role of helping faculty find the right tools for their research. In some cases, particularly with ChemSpider and the Chemical Data Service, academic librarians are aware of the services, but in others, their knowledge of the latest research technologies is incomplete.

While some of the information services that chemists use are funded by grants or business models that do not involve direct charges to academic institutions, these resources also place strains on the budgets of academic libraries. Libraries are also limited in their ability to purchase new products. As chemistry research continues to progress, and interdisciplinary and sub-field publications continue to be introduced, libraries are struggling to maintain a balance in the collections between core resources and new journals and technologies.

Tools for Discovery

Electronic publishing has changed the way that chemists find and read content published by their peers and colleagues. There has been a general shift from reading to searching that has had implications for the ways that work is done and new generations of students are trained. While search tools have eased the research process for most scholars, there are still other modes of discovery in which they are underserved. Specifically, chemists frequently feel overwhelmed by the volume of new publications in their field, and the search tools available to them now do not enhance their ability to stay abreast of new research on an ongoing basis.[5]

The two modes of discovery that are important to chemists are active searching and passive awareness of the current literature. Each of these is supported by different types of information services. The survey asked respondents about each of these modes, and found that they rely on very different types of tools. When looking for information or research articles, chemists heavily prefer chemistry-specific search engines along with general purpose search engines. However, the set of resources that they rate as being most important to learning about new research are different. Search engines are still very important in learning about

5 Our findings confirm many of the conclusions of the Research Information Network (RIN) in its case study on chemistry: Research Information Network, *Collaborative Yet Independent: Information Practices in the Physical Sciences*, December 2011, http://www.rin.ac.uk/our-work/using-and-accessing-information-resources/physical-sciences-case-studies-use-and-discovery-.

new research, but so are review articles, conferences, and conversations with colleagues, all of which allow chemists to learn about new research without having to actively go out and look for it (see Figures 2 and 3). Interviewees' comments about the difficulty of keeping up with current research suggest that there is room for improvement in these passive, serendipitous discovery mechanisms, which do not currently take advantage of new technologies.

FIGURE 2

When you explore the scholarly literature to find new journal articles and monographs relevant to your research interests, how do you most often begin your process?

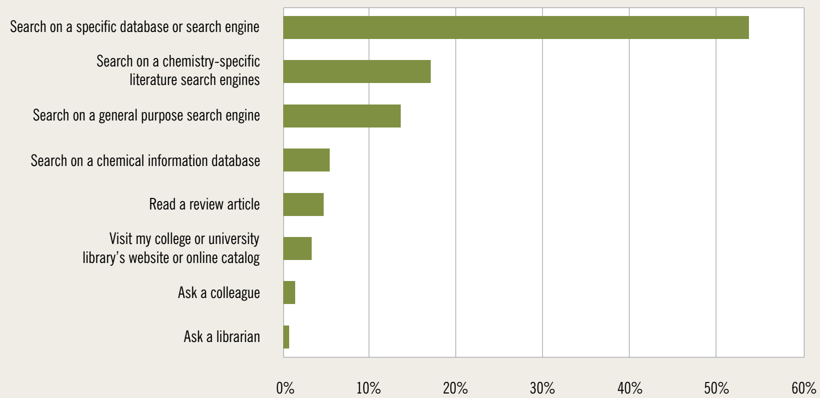
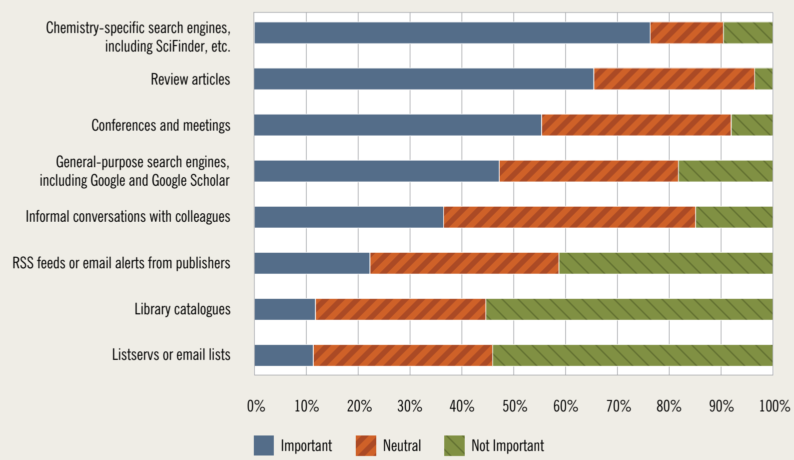


FIGURE 3

How important to you is each of the following as a means of learning about new research?



Changes in Modes of Discovery

Most of the interviewees expressed a deep anxiety about "keeping up" with all of the relevant research being published in their specialization. The way that chemists interact with scholarly literature has changed dramatically since the widespread uptake of online publication. Most interviewees who graduated before the age of digital journals reported that they used to visit the library once or twice a week to look through all of the new journal issues that had arrived. This forced them to set aside time to read the literature, and it was sometimes also a social activity that they would do with colleagues. With the growing number of publications, most chemistry scholars now feel that they do not have the time to leaf through all of the journals that are relevant to their field. Instead, they rely heavily on email alerts and RSS feeds from publishers, but they rarely have time to read these, either. The deluge of new journal articles has been met on the other hand by drastically improved tools for searching through the literature. These tools have enabled chemists to make a broad shift from reading to searching, an important change with consequences for researchers, libraries, and publishers.

Senior scholars identified a number of other minor results of this shift toward search: the loss of serendipitous research finds and a generational shift in the way that chemists look for information. Older scholars also felt that they have lost the serendipitous aspect of flipping through a journal and discovering something of interest to them that they would never have found through a keyword search. Now it is impossible to spend an afternoon at the library reading through a journal: "You're overwhelmed with huge amounts of work and everything needs to be done quickly, so you just cannot take the luxury anymore to spend that much time." Some senior scholars are under the impression that their students' focus on searching for information means that they do not spend enough time absorbing information from articles and engaging with the literature in their field. "Journal clubs" are a common remedy for this; they bring together chemists and their students, sometimes from around the department, to discuss recent research. One professor said "When I was a student, everybody went to the library for half an hour and looked at the literature. These days, they—it's hard—some students, it's extremely hard to get them to read the literature. They just want to Google everything." Conferences are now seen as one of the easiest way of keeping up with current research, because they provide a distilled introduction to other researchers' work. They give a condensed introduction to research that can be difficult to find elsewhere.

Finding Content

As explained above, journal articles have remained the most important type of publication for chemists, but because of the ease of searching, journals have become much less important as curators of content, even if they retain their role as a signal of a paper's quality: "To be honest, one reads papers based on the science that's done in them…I don't tend to go to a journal site and look at what might be there. I go to a journal site because I'm after a particular paper." Of course, this is not true of all chemists; many researchers regularly check the websites of key journals to find new content in their area of specialization. Only a few researchers said they regularly follow general science journals like Nature and Science, while other chemists said they ignore these publications because they so rarely publish articles from their specialization. The assumption that chemists are more likely to page through "brand name" journals appears to be breaking down. While it is still regarded as a great honor to be published in one of these journals, many chemists disregard them because they have so much content that is completely outside their area of interest.

A common means of staying updated is through following journal table of contents email updates or RSS feeds, as well as setting citation alerts for key phrases or researcher names. Chemists are frequently overwhelmed by the amount of email that they get from publishers, but they feel that this is their best option for keeping current. Many researchers have citation alerts set up for their own names and for certain key phrases, so they can track the newest work in their specialization. Some mentioned that they closely monitor other labs that work in their specialization. This method is sometimes imperfect because name authority control can be a problem—sometimes there are variations on name spellings that make it harder to find content. At least one researcher said that it would be helpful to have a better tool to help process all of this information, something that what would "do a pre-scan of things like announcements that come from journals… I have 1,410 of them which are unread."

The main destination search sites for chemists are Web of Knowledge/Web of Science, SciFinder, and PubMed. Most researchers use one or more of these sites as their first destination when they are searching for journal articles. Structure-based searching has enormously improved the ability of researchers to get information about molecules of interest to them; it has been especially useful for synthetic chemists. SciFinder and other databases prioritize visual browsing of articles, because this is the easiest way for a chemist to scan an article and judge its relevance. Most chemists said that they use Google in their research, but few of them use it as a primary destination. Instead, they usually start with a chemistry-specific resource and then resort to Google if they can't find anything. In the words of one professor, "It's never a search engine of first choice…if I'm using it for work related stuff, it's more likely to be teaching than research." One researcher said that he uses Google at "the fuzziest level of researching things" (i.e. when he is exploring a new area and using non-specific search terms).

Literature and Research Notes Management

Much as they did before the advent of electronic publishing, chemists still keep personal collections of papers that they intend to use in their research, though they do not always have the right tools available for organizing them. Chemistry labs produce large volumes of notes and documentation that must be stored for future reference, but these are largely kept in paper format. Electronic lab notebooks have yet to make a substantial impact on the ways that chemists work. Librarians and other campus-level service providers have not taken on the role of promoting or supporting the use of ELNs.

Article Collections

Most chemists maintain a collection of journal articles as PDFs saved on their primary computer. They add to this as they encounter new articles that they might be interested in, filing them in folders based on subject matter and assigning them filenames that will make them easy to locate later on. The maintenance of a personal collection of research articles seems to be a digital holdover of the way that chemists worked in the past. One researcher said that she always kept a filing system with photocopies of all of the pertinent research in her field, though she gave up on this gradually as electronic versions became available.

A few interviewees said they use a tool such as Mendeley to maintain these collections and make them searchable, but for the most part chemistry researchers have very simple and remarkably uniform practices for saving articles. EndNote has become a basic research tool used by many chemists, though there are many chemists who find it cumbersome and go without it. Some chemists use it as a makeshift citation database.

Electronic Lab Notebooks

Many chemists are attracted to the idea of Electronic Lab Notebooks (ELNs) because they promise to solve key problems of research notes management and collaboration within lab groups. By making it easy to share, archive, and search through past lab notes, they could ease some of the current research management challenges posed by paper format lab notebooks. Grants often require the retention of lab books, but this is almost never monitored because it would be so difficult to verify anything with paper notes. As lab leaders become more and more focused on their administrative duties, they have little time to review students' lab books, so while they often keep these books after their students leave, they are not familiar with what they contain, and the information is not indexed in any way. ELNs hold out the promise of making lab books easily shareable and searchable, eliminating some of the problems of traditional paper format lab books. They might make it easier for more researchers to adopt the principles of open notebook science.

The primary problem with ELNs, which was mentioned by almost all chemists who do not use them, is the challenge of protecting electronic equipment in the lab. Many lab leaders feel that there is too great a risk in taking computers or tablets into the lab, where they could easily be damaged if an experiment becomes messy. (Most chemistry labs have a separate office area where students can do their desk work. In many labs, computers are not allowed in the lab space at all.) Instead, some chemists have developed workarounds that make it easier to share information from their paper lab books. For example, one leader said that he takes pictures of key pages from his students' lab notebooks at the end of the day so that he can review them later. There are also concerns that ELN software is not sufficient to meet chemists' needs; they have been called promising for a decade, but they have not been implemented successfully in that many labs. Only 21% of survey respondents reported that they had used an ELN in their research, and those that had experience with them had mixed opinions of their usefulness. One interviewee who was part of a pilot project a decade ago said that the system failed because the software and hardware were not yet advanced enough; his lab lost data because of slow wireless internet connections.

In computational chemistry, ELNs are more practical because there is no risk to the equipment and because researchers and their students do most of their work on computers already. We found a range of opinions about ELNs among computational chemists and others who do not often do "wet chemistry" research. Some have found the transition to electronic research notes much more seamless. However, many of these labs are using widely available word-processing applications or cloud services like Google Docs rather than special lab note management systems. One computational chemist said, "The system I really like…is to maintain two shared Google documents. One is to record what they did and the other is to record what they're planning to do." However, other researchers said that they are actually less diligent about taking notes than colleagues who work in the lab. "Computational chemists tend to expect things to be self-documenting…so they're much less systematic about recording what they're doing and why at a particular time, which sometimes means that in terms of thinking about sharing that stuff afterwards, that causes a big problem." ELNs hold more promise in computational chemistry labs because they could add some automation to the process of keeping research notes, though several interviewees said that they have not yet seen a product that offers this feature to their satisfaction.

Managing and Sharing Data

There is a growing consensus that openness is in the service of science, but managing and sharing data is a complex process that must be carefully managed. In its report Science as an Open Enterprise, the Royal Society wrote, "Realizing the benefits of open data requires effective communication through a more intelligent openness: data must be accessible and readily located; they must be intelligible to those who wish to scrutinize them; data must be assessable so that judgments can be made about their reliability and the competence of those who created them; and they must be usable by others."[6] Current data management practices in chemistry are sub-optimal, and while chemists frequently share data, they do not always do so publicly. In the wake of new requirements imposed on academics by private and public funders, many researchers have begun to express increased demand for support from their institutions.

Data management

Chemists have a general lack of awareness of what constitutes effective data curation and preservation, and they often choose not to use the IT infrastructure that would enable them to manage data more effectively. They are unaware of what they are required to keep, and they do not always create the appropriate metadata to help others interpret their work. While funders' data retention policies have made chemists much more mindful of keeping their data, they are still often unaware of specific requirements and they do not closely monitor their compliance. Most of them have a general idea how long they should keep the data, but they do not pay close attention to the different policies at various major funders, especially when they have multiple projects and several sources of funding.

There is an assumption, in the words of one researcher, that "most chemists are reasonably IT literate," but we found that most chemists do not have the time or inclination to closely monitor data management in their labs. Many feel they have already dealt with this issue in full; 51% of survey respondents agreed with the statement, "My research data is properly preserved and documented for access in the future." In many ways, chemistry labs are left to create their own IT infrastructure with little funding or oversight from their departments and universities. Labs generally do not have good data management infrastructure or proper external support for developing it.

6 The Royal Society Science Policy Centre, *Science as an Open Enterprise*, June 2012.

When it comes to sharing and preserving files, many labs either lack or choose not to take advantage of IT infrastructure like shared network drives and data repositories. Rather than using the university's network, lab members transfer files between computers by emailing files to each other. Some have started to use cloud services like DropBox. These services provide a convenient place for groups to seamlessly share their work internally as well as with outside collaborators. However, they can also be costly and they could present security risks. The data preservation services that universities offer generally come with fees based on usage, and this has created a powerful disincentive to safe data management. Chemists generally opt to keep their own files on DVDs or external hard drives, which are cheaper than institutional data storage services. At some institutions, even the shared departmental labs opt not to use institutional data storage because of the extra cost. One chemist told us that at her institution, the cost of university disk space is over £500 per terabyte per year. In computational chemistry, it can be very difficult for researchers to keep all of their data because it is often on the gigabyte scale for every one of their projects, so the fees become impractical.

Research data is most often managed by individual students or postdoctoral scholars, and since these populations are highly transient, there is little continuity in the way that data is stored. Several researchers said that they ask their graduating students to give them all of their data on CDs, DVDs, or external hard drives. This introduces the risks of technological obsolescence or physical damage to the storage equipment; one professor said that he had nearly suffered a serious data loss when a student reformatted a hard drive containing research data from a former student. Luckily he was able to recover the data by contacting his former student. Another interviewee said that he has old data files that would be difficult to access now because they are in obsolete formats, so it would be easier for him to just repeat the experiment. This piecemeal approach also makes it difficult to locate data, since information is arranged by lab member rather than by subject area. Several researchers who currently keep all of their data in complex folder systems said they need better ways to search through their data comprehensively. Database products designed around the needs of chemistry labs might be able to meet many of their needs, but they have not had the time or funds to implement them.

In many shared departmental labs there is duplicative storage of data, with the researcher keeping his or her own copy and the technician or department storing another copy centrally. This occurs with shared equipment like mass spectrometers, but it is also the case for computational chemists who use high-performance computing facilities, which also sometimes have their own backup systems. In many cases, one or both copies of the data have insufficient metadata attached to them, causing them to be of little use to anyone else. Thus, while much of the necessary data is being stored somewhere, it is kept in a way that is of questionable value and yet is still very resource-intensive. Data delivery from specialized labs is sometimes crude as well: data from the EPSRC Institute of Mass Spectrometry at Swansea University is delivered by email. The National Crystallography Services is in the process of setting up an automated system that will allow researchers to log in and download their CIF files. Some institutions have already implemented data server systems like this one at a local level, but this progress is uneven.

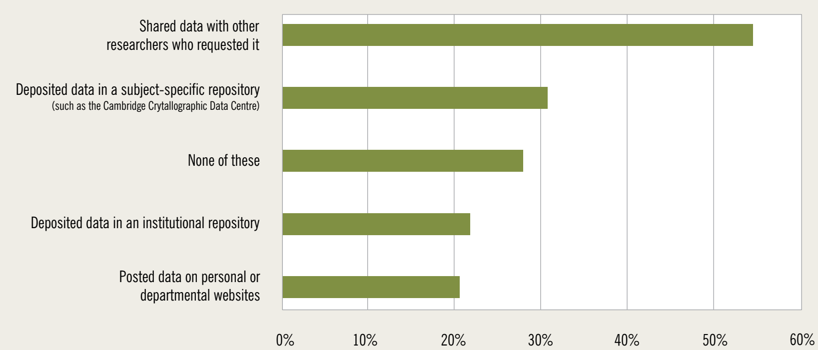
Some researchers were very conscious of their need for better data management and better IT infrastructure. One chemist, who currently has his students manage and back up their own crystallography data on their individual computers, reflected on his lab's need for better data management: "It would be very useful, you know, if I had a free IT person who just…helped me out and set all that stuff up and could maintain all that and make sure there were no problems. That would be fantastic, because we'd have very easy access to all of the archived data, which over time becomes progressively difficult to access." However, chemists do not have anywhere to look for this help right now, and the library was not the first place they would look to find it.

Sharing Data

There are still a broad range of opinions about the utility of sharing data in chemistry, and the discipline has yet to develop systematized and widely adopted standards for how and when researchers should make their data available. The existing data sharing ecosystem relies on informal sharing between scholars, deposits in subject-specific or institutional repositories, and the publication of data as supplemental materials alongside journal articles on online platforms. Chemists often share data with their peers when they are requested to do so, though they are less likely to post their data in an online repository. A majority (54%) of the chemists who responded to the survey said that their lab had shared its data at the request of another researcher. While 28% of respondents said that they had not shared data in any of these ways in the past year, many others reported that they share their data in several different ways (see Figure 4).

FIGURE 4

In the last year, have you or your research group made any of your data available in any of the following ways? (Please check all that apply.)



Many chemists still do not like to share their data publicly. The data that they produce sometimes has potential economic value, and unless they are under an obligation to share it, it is not always in their best interest to do so. In the interviews, many chemists said that they like to have close control over when and how their data is shared. According to one researcher, "Most chemists are fairly defensive about it. I would say that most people here would not be open to the idea of immediately sharing data after it was published." Chemists also question the value of trying to make their data intelligible to the broader public. In the words of one chemist: "I can make my raw data available, but it's not going to mean anything to anyone in the public. So am I then going to be asked to make it available in a form that's viewable?" Journal articles in chemistry are much closer to the data than those in other fields; they are often very short explanations of data, rather than longer explorations of a topic that draw on data. Therefore, in some cases it may feel redundant for a chemist to go back and try to explain the data in yet another format. Despite reluctance to share on the part of some researchers, there was general acknowledgement that some data sharing, in whatever form that might take, has the opportunity to enable significant advances in chemistry research.

The EPSRC has set data sharing guidelines that strongly favor openness. The first principle of its Policy Framework on Research Data states, "funded research data is a public good produced in the public interest and should be made freely and openly available with as few restrictions as possible in a timely and responsible manner." It also points to the importance of appropriate metadata, and it recognizes data management as an appropriate use of grant funds. However, it also acknowledges the rights of researchers to "a limited period of privileged access to the data they collect" and notes that not all data will be appropriate for public release. It is difficult to quantify the exact impact that this policy has had in chemistry.[7]

Responsibility for supporting data management and preservation oftentimes falls between the traditional responsibilities of the various campus departments. Libraries, which are often responsible for institutional repositories, are not always equipped to meet faculty members' needs in this area, and among our interviewees there were differences of opinion about what role they should play. Many of the subject librarians who we interviewed were eager to be included in the discussion about data management on their campus, but they noted that working with faculty data requires expertise beyond what most library staff members are trained to provide. Many institutions have campus-wide or departmental initiatives exploring the best ways to provide robust support for data management.

Many UK universities and colleges have implemented some version of an institutional repository to collect and disseminate the scholarly output of students, researchers, and faculty.[8] These institutional repositories are often used as a means of facilitating the collection of research publications mandated by the Research Excellence Framework process. In some cases, they are also being used to store and share researchers' experimental data, as specified in a data management plan. However, institutional repositories are often built with research publications in mind rather than data. Many librarians said that their repositories are not set up to store large datasets, so the technology imposes limitations on faculty who might want to use them to share data.

There are also several examples of cross-institutional online repositories in chemistry. The Cambridge Crystallography Data Centre (CCDC) and the field of crystallography in general provide the best example of successful data standardization, sharing, and archiving in chemistry. The standard .CIF format allows researchers to easily take advantage of each others' data. Most publish-

7 "EPSRC Policy Framework on Research Data: Principles," Accessed 1/25/13, http://www.epsrc.ac.uk/about/standards/researchdata/Pages/principles.aspx.

8 UKOLN: Digital Repositories Review, 2005. http://www.jisc.ac.uk/uploaded_documents/digital-repositories-review-2005.pdf.

ers make it mandatory that the data associated with articles in their journals be deposited with the CCDC. However, even with the CCDC, there is no standard procedure for how and when researchers make deposits. Some researchers send data on crystal structures that have not been peer reviewed and published, while others wait until publication. Some of those who wait until they publish choose to submit their own data at the beginning of the publication process or ask a lab technician to do so on their behalf. In other cases, the journal publisher will manage the deposit for the researcher. The newly consolidated National Chemical Database Services may soon make it easier for researchers to share their data.

While chemists have not been as quick to share their data as researchers in other scientific fields, they almost always submit them to publishers as supplemental materials, and publisher databases have come to be seen as de facto repositories. The articles themselves are often the best descriptors of the data, so there are significant benefits to placing the article and the related data on the same platform. These materials are often freely available, even when the articles they are related to are not. Several chemists went as far as to say that they consider their published supplemental data to be sufficient backup for their own files: "There's a limit to how much you really need to keep, and we do keep it on CDs and things, but… all of the data that actually go into backing up the paper will get deposited with the journal anyway." However, librarians and chemists pointed to several major flaws that make this a less than ideal way to store data. First, publishers do not always manage data collections in a way that maximizes scholars' ability to reuse research materials. Oftentimes they store data in inappropriate file types such as PDFs, or they do not attach the appropriate metadata. Second, the data that authors submit to journals is sometimes incomplete or lacking in necessary details. Finally, publishers do not typically commit to storing and hosting data in perpetuity.

Research Dissemination

Chemists publish frequently and they are strongly committed to the traditional structure of journal articles. Like other scientists, they use publication to push their ideas out into their research community, but they also use articles as a means of entering their data into the scholarly record for future researchers. Chemists do not have a strong commitment to open access publication or to sharing most of their data, in part because of the competitiveness of the field and in part because chemists rarely have trouble getting access to the materials that they need.

Publication Practices

Most of the lab leaders we spoke to said they like to publish at least 3-4 times a year. Survey respondents gave widely varied estimates of how often they published, but the average number of reported publications over the past three years was 16. Younger scholars learn about where to publish by doing their own background research on the journals in their specialty and by talking to their colleagues. "You need to do a little bit of research about the journals and how they are perceived and what kinds of articles they normally publish and how…the whole peer review process goes." Chemists do not typically look to their libraries for advice about how and where to publish. A large majority of survey respondents (74%) said they have consulted fellow academics about this, but only one respondent said that he or she had talked to a librarian about this issue.[9]

The HEFCE Research Excellence Framework (REF), which requires scholars and institutions to submit extensive reports and evidence of research outputs for review, has played a significant role in shaping chemists' publications strategies. Institutions want to show evidence of highly impactful publications, and researchers in turn feel pressure to publish in well-regarded journals. In chemistry there is a rigidly hierarchical journal environment in which most scholars try to publish in top journals like Nature and Science, followed by the top chemistry journals, and then more specialized journals within chemistry.[10] Most of the interviewees confirmed this dynamic, and said that it is reinforced by tenure practices and the Research Excellence Framework, both of which assign higher value to journals that are farther up in the spectrum of publications.

In many areas of chemistry, publication acts as the archival vehicle for researchers' work, and this is a major motivation to publish. The article ensures that the researcher's work is archived and the associated data is made available. For example, a chemist who publishes about a crystal structure will have their .CIF data archived at the CCDC and his or her article will be searchable to future chemists. The information contained in databases of chemical information is pulled from the published literature; this makes journal articles the best way to disseminate information. Semantic chemistry may someday be able to simplify the time-consuming manual process of creating these resources. As Velden and Lagoze write, "The problem would be eased if the authors, who have the best domain knowledge with regard to their own publication, would contribute to the mark-up of chemical information, and would be enabled to do so painlessly with easy-to-use tools." This innovation would obviously result in a much broader transformation of publication practices, but for now journal articles remain paramount.

Review articles, which sum up all of the important recent research on a topic, are very useful as research tools, but some chemists regard them as being less important to a researcher's career than articles presenting original research.. Review articles are a useful entry point into the literature because they help researchers understand the trajectory and context of original research articles. They play an important role in introducing chemists to new areas of research in a simple and less time-consuming fashion. However, chemists publish them much less frequently and some stay away from publishing them altogether. In the survey, respondents reported publishing an average of 1.6 review articles over the past three years, compared with an average of 16 original research articles. Nearly a third of respondents said they have not published a review article at all during that period. When they are writing review articles, chemists use a very different set of skills than they would typically need for a research paper. Writing a review articles requires a lot of "library work"—i.e. bibliographic work. They are sometimes regarded as a good "first publication" for graduate students because

9 The full text of the question was: "With whom would you be most likely to consult about where to publish an article and how to work with the publisher?"

10 Theresa Velden and Carl Lagoze, *The Value of New Scientific Communication Models for Chemistry*, 2008, http://hdl.handle.net/1813/14150, p. 26.

they do not need to be attached to any ground-breaking original research. Many chemists use the information that they have gathered in a literature review for a research project to assemble a review article.

A few researchers said that they think chemists publish too much, and that the field would benefit greatly if there were less pressure to publish frequently, because then researchers could spend more time working on high-quality, high-impact articles. Many librarians echoed this sentiment; according to at least one interviewee, "There are too many journals." This perception seemed to touch on all aspects of the publication cycle–there are too many journals to publish in, there are too many journals to purchase, there are too many places to find the journals, and there are too many journals to read. Some believe that this situation is building toward a tipping point, when there will be a major change in the publishing model in chemistry, but this was not the majority opinion among interviewees.

Chemists are fairly "traditional" when it comes to scholarly communication; they have been slow to embrace new forms of sharing information about their research results. Several of our interviewees mentioned using new forms of media. One interviewee mentioned that she has a colleague who uses Twitter to write about her research, but acknowledged that this is difficult to do in chemistry, because it is considered unwise to share too much of your results. This method of sharing is more appropriate for large public research projects. Another example came from a chemist who said that he would like to have an online, interactive component to the book that he is writing, "which may well look like a Wiki in this form or maybe some kind of self-contained website tutorial." However, he is not interested in releasing more information about his work, because he worries about getting bogged down by questions from other researchers who are trying to reproduce his methods.

Peer Review

Chemists take on a variable amount of peer review work, depending on their specialization and career stage. Most of the researchers we spoke with were content with the peer review process and their role as reviewers, and the review process can play a very important role in the scholarly communication ecosystem. One researcher commented that, within his smaller sub-discipline of chemistry, the anonymous interactions that researchers have through the peer review process for grants and publication are an important part of scholarly communication. A handful said they would like to see more experimentation with alternative models; for example, one chemist said she wishes that there could be open peer review. A handful of interviewees said they have stopped reviewing articles for for-profit publishers, either because they are ideologically opposed to them or because they see little benefit in doing the work. One researcher said, "As some compensation for reviewing of journal articles for particular journals, it was common to provide hard-copy journal subscriptions. This has been replaced recently with access to electronic versions, which for me is just useless because I have this through the university." One the other hand, chemists expressed stronger loyalty to the RSC and the ACS because they view them primarily as scholarly societies and non-profit organizations.

Open Access Publishing

Chemists are relatively ambivalent about the issue of open access publishing. Our interviews suggest that most chemists do not experience significant problems accessing the content that they need, and they see little need for their content on the part of the public. Consequently, many of them are either agnostic on the issue of open access to research outputs or have only lukewarm support for it. However, many of them have begun to prepare for new regulations on the issue. Several of our interviewees mentioned that they have already started to include funds for open access publication in their budgets for grant applications.

The long-term impact of new regulations in support of gold open access publishing is still unclear. The Report of the Working Group on Expanding Access to Published Research Findings ("The Finch Report") advised a much stronger support of gold open access publishing on the part of funding bodies in the UK. One of the key issues in the implementation of such a policy for chemistry would be its relationship to the REF. Chemists told us that because of the REF, they feel that they are under great pressure to publish in prestigious journals. This might counteract some of the increase in competition that the working group hopes will put downward pressure on the price of scholarly publishing: "We expect market competition to intensify, and that universities and funders should be able to use their power as purchasers to bear down on the costs to them both of APCs and of subscriptions."[11]

Academic chemists rarely have serious trouble getting access to the papers that they need, and they know the same is true for many of their colleagues, so they do not see how paying to publish open access would improve access for the people who need the research most. One chemist said: "I think it's very expensive. Most of the universities have—they have the subscriptions so they have access to it. It's probably a bit of an issue for the more developing countries." Many chemists also take issue with the idea that the public needs access to their articles, because unlike research published in some other fields, it is difficult or impossible for the general public to understand it. Most trained chemists are either at an academic institution or a company with the means to purchase access. Another professor argued: "It's a waste of research money, I think, because the only way we could do that would be to include vast sums onto—or what I would consider vast sums—onto research grants…And I really don't think the public are going to go to a chemistry journal website to look up an article."

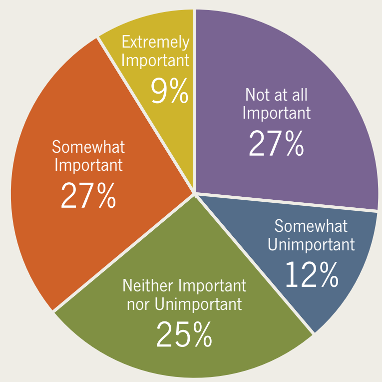
Chemists are particularly wary of paying to publish in journals that they have published in for years for free. Recent library budget cuts have made them strongly aware of their library's collections budgets, and some researchers are reluctant to pay publishers to make their articles open access when they know that it has little short-term effect on the costs of the journals to their library. One researcher asked, "Surely we ought to get some money off the price of the journal, shouldn't we?" Similarly, chemists are sometimes also dismissive of publication services that cost extra money, like color figures or paying to be on the cover of a journal. Every researcher has his or her own strategy for choosing journals, and sometimes these strategies take into account access issues. In our survey, 9% of

11 *Accessibility, sustainability, excellence: how to expand access to research publications*, June 2012, Working Group on Expanding Access to Published Research Findings.

respondents said that it is extremely important to them that the journals that they publish with make their content freely available, and 27% said that this issue was not important to them at all. This means that the majority (65%) do not feel very strongly about the issue (see Figure 5). For example, one chemist said that while she does not favor open access journals, she does try to publish in journals to which her own institution has access.

FIGURE 5

When it comes to influencing your decisions about journals in which to publish an article of yours, how important to you is it that the journal makes its articles freely available on the internet, so there is no cost to purchase or read it?



On the other hand, not all chemists see fully open access journals as a good venue for publishing their research. The REF and tenure review processes have created a bias against open access journals in chemistry by focusing researchers' attention on journals' impact factor, and has thus driven them away from open access publications, which until recently have had lower impact factors. As one researcher said, "I want my work to be published in the best possible journal with the highest impact factor and [where] its most likely to be cited, and whether it's open access or not, I just don't care, quite frankly." Another chemist echoed this sentiment: "For me, it's about the quality of the journals. I don't really mind if it's open access or not. …it's all about publishing in the appropriate journal that suits the quality of my work." One interviewee who had published in an open access journal said that he had been dissatisfied with the number of citations that the article had attracted, and he attributed this in part to the low impact factor of the journal. This trend may change as some open access journals' impact factors improve.

Online Repositories

Chemists are not heavy users of institutional and subject repositories for research articles. In the survey, 67% of respondents reported that they have never deposited any of their publications in an online repository. Of those who have deposited their work, a majority (67%), said that less than 40% of their total published output was available in one or more repositories. However, many interviewees suggested that they are receptive to the idea of using them, especially if their institution mandates it. Some chemists who support open access like the idea of using repositories as an alternative to a pay-to-publish model. One interviewee said that she likes the idea of creating a convenient collection of her own papers: "Having a repository for one's papers in one place in a way that you could just pick them would be a nice thing, from an archiving point of view." Some institutions have used their repositories to organize the information that they need for the REF by requiring faculty to submit copies of their research publications (or at least the citations, in cases where copyright prohibits more than that) in the institutional repository. Many publishers, both for-profit and non-profit, allow publishers to self-archive after a certain amount of time has passed since an article's publication. The ACS and the RSC, for example, both allow authors to self-archive their published work in a repository 12 months after its publications, and several of the major commercial scientific publishers have adopted similar policies as well.

Research Funding

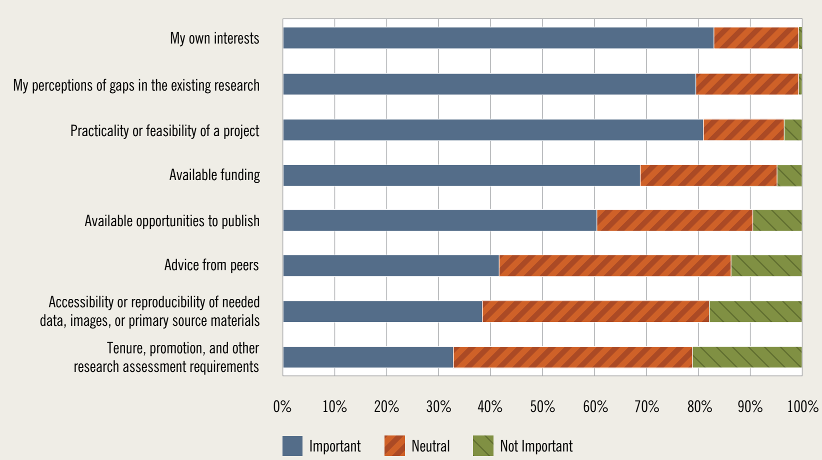
Public funding from the EPSRC remains the most important source of money for chemistry research in the UK, and the Council's policies have enormous impact on the type of research that chemists choose to pursue. Collaboration with industry can also yield funding, though usually only for applied research. More chemists are looking for industry funding as public funding is cut back.

Public Funding

In respect to funding, our conversations with interviewees were narrowly confined to researchers' personal experiences with the primary public funding body for chemistry in the UK, the Engineering and Physical Sciences Research Council (EPSRC). Their opinions confirmed the power of the EPSRC policies to shape the future of chemistry research in the UK and demonstrated the impact that they can have on individual labs' working practices. In the survey, respondents ranked the availability of research funding as the fourth most important factor in choosing a research topic, with 69% saying that this was important to them (see Figure 6).

FIGURE 6

When you think about new research projects or areas, how important is each of the following in helping you define and select the areas to pursue?



EPSRC policies have a direct effect on the way that chemists frame their research plans. For example, several chemists mentioned that the EPSRC had helped guide them toward interdisciplinary research. One researcher said that an ESPRC interdisciplinary grant program had actually helped change his opinion of working with non-chemists, because his past project had been so successful. Another interviewee noted that it is easier to get interdisciplinary funding than it used to be, because RCUK have made policy enhancements to streamline this process. EPSRC policy changes emphasizing economic impact have already changed the way that chemists think about their work. One interviewee mentioned that during his last project, he secured a letter of support from an industrial collaborator to support the claim that his research might have long-term impact on their industry. Another professor mentioned that he is looking for engineers who will collaborate with him and apply some of the materials that he has developed, in order to prove that his work has practical applications.

A few researchers questioned the funding directions of the EPSRC. One professor said that one of the biggest challenges in his lab is finding high-quality graduate students, a problem that he thinks will intensify as the result of the EPSRC's decision to focus on Doctoral Training Centres rather than funding students at a broader set of institutions. Other researchers complained about how it has been more difficult to get EPSRC funding for research equipment. While EPSRC funding is sought after at all institutions, researchers who have had research money from other sources find it to be comparatively difficult to deal with. One chemist described the funding process as "stifling." "The whole process has been very bureaucratic…the amount of hassle per pound has been tremendous compared to any other money that I've ever had before." Chemists are keenly aware of the increasing difficulty of obtaining funding for their research; 61% of survey respondents agreed with the statement, "It is increasingly difficult for me to find government or charitable funding for my research."

Industry Funding

As government funding has become very competitive, researchers have increasingly looked to industry to make up for the lack of funds. Many chemists expressed an interest in collaborating with an industrial partner, with 67% of survey respondents agreeing with the statement "I have a strong interest in collaborating on projects with industry." This is probably in part a result of the funding environment and increased focus on the commercial impact of academic research. With these changes, university research offices have become a vital source of support to many faculty members who are negotiating new relationships with the companies that fund them.

Chemists at institutions that are not top-ranked told us that they have more success finding funds for applied research. One researcher said, "We're…not a high-ranking institution in terms of research in the UK. It's sort of mid-ranking, and so getting money from commercial sources is actually easier than from the UK research councils." Smaller companies can be natural partners for chemists at universities that are not top-ranked. They have less money to spend on internal research and development, and they have specific problems that chemists in academia can help them solve, but researchers at larger departments are less likely to work with them because they do not do as much applied research. Funding a graduate student is a relatively accessible way for businesses, especially smaller ones, to connect with a lab and begin a research project relevant to the business' needs.

One chemist said that he would value more opportunities to meet with representatives from industry, and he thinks that the RSC could play an important role in making these connections, though he said that in the past, the RSC has seemed to focus on large chemical companies, not the small to medium sized companies with which he is looking to partner. Some researchers expressed fears that the REF will underestimate the impact and importance of industry collaborations, even while the UK government is trying to encourage this collaboration.

University offices for research, commercialization, and intellectual property management have become very important service providers in this new funding environment. At some institutions, research offices help chemists prepare grant applications and estimate budgets. Most universities also maintain spinoff offices that deal with intellectual property issues related to the work of faculty members. These offices will review project proposals to gauge whether there is potential for commercialization, help researchers identify potential industry partners, and provide advice along the way. However, this remains a relatively rare way to make connections in industry. Only a handful of chemists who responded to the survey (5%) said they had been introduced to an industrial research partner through their universities' intellectual property offices; the vast majority established their industry connections either through personal or professional acquaintances or after a company approached them directly. Several chemists said that their research offices had been enormously helpful in putting together grant applications, but one noted that managing relationships with outside companies can be delicate work that requires careful coordination. While the university can act as a catalyst for collaboration with industry, it can also impose too much pressure on the working relationship: "There's often a balance to be struck there between… trying to encourage and support the business to work with the university, but not giving them so much attention that it sort of puts them off."

Recommendations

Based on our findings we offer three major recommendations that are solidly within the scope of this project. We have attempted to frame each recommendation in an unambiguous problem statement derived from the project's findings and the broader environmental context. Following this problem statement, we issue our core recommendation. Finally, we offer several opportunities for new service models as options through which our recommendations might be realized; these are not intended to be recommendations but rather to inspire innovation, design, and prototyping as appropriate within the context of a given service provider.

We recognize the difficulty of implementing the service model opportunities we have identified, especially at the level of an individual university. Our recommendations are based on an assessment of the needs of chemists, and we are confident that they represent compelling ideas for new services. Scholar-centric services innovation will require, at times, a willingness to collaborate beyond traditional organizational structures or deploy new types of staff skills and expertise. In some cases service providers have already begun to work toward some of the solutions that we suggest below.

Research Management Services

Problem statement: Chemists require better knowledge management infrastructure, systems, and training.

Chemistry lab groups are complicated working groups with interlinked responsibilities, and it can be challenging for them to manage their research notes and data collaboratively. We observed some creative solutions to this challenge, such as senior researchers who take pictures of all of their students' lab notebooks at the end of every day. Chemists have sub-optimal data management and preservation practices. Because they often work in large lab groups, it is difficult for academic chemists to coordinate the recording of data during the experimental process and the preservation of that data after the completion of a project. When data are saved, they are often held in unstable or at-risk formats (such as removable hard drives, CDs, or DVDs) or in formats where no one else can access or interpret them (in lab books). Sometimes most of the useful data are included with the final published outputs, but, at other times, a large amount of potentially useful data is not shared or preserved in any durable way. During the interviews, many chemists said that they do not pay close attention to data management and preservation beyond what is required by their funder. Chemical informatics specialists often see electronic lab notebooks (ELNs), along with some of the associated technology, as one of the best solutions to these problems. While most chemists understand the potential benefits of using Electronic lab notebooks, few have adopted them in their labs. Survey respondents expressed a somewhat ambivalent view of them, with only 13% of those who had tried them saying that they were very satisfied with them. Many of the interviewees said that they like the idea of using ELNs, but they do not have the funding to buy the necessary equipment or they worry about keeping the equipment safe in the lab.

Recommendation

Institutions and funders should assess the data management needs of chemistry research groups and ensure that they have access to the appropriate infrastructure, systems, staff, and training. The proper management of research data requires a substantial commitment of time and resources; funders should encourage chemists to recognize this in their funding requests and universities should make provision for it in their staffing. New tools and processes, recognizing how data are and can be managed in the research processes of chemistry laboratory groups, are needed to ensure that valuable data are appropriately preserved and shared.

Opportunity 1: Knowledge Management Tools and Processes

Too often the lab leader is the only member of a lab group who knows about all of the lab's activities, and he or she becomes a single point of failure for all the team's work. Labs should develop better protocols for sharing information, data, drafts, and ideas. Software providers should build tools that adapt to the team structure of chemistry labs and enable the free flow of information. ELNs have not yet evolved to the point of being widely adopted, even though many chemists have experimented with them. While many researchers commented that the technologies have improved, they are still not compelling enough to present a clear value proposition to their owners, to some degree because their focus is scoped too narrowly. ELN producers may wish to redevelop their offerings so that they reduce some of the pain points associated with knowledge management in chemistry labs, especially as they relate to data management.

Opportunity 2: Institutional Data Management Assistance

Few institutions offer intensive guidance on data management or assistance with data curation and storage, and few chemists consider this to be a core part of their research process. Data management and preservation is time-consuming and rarely straightforward; it requires expert advice and constant monitoring. Universities can significantly support chemists by devoting specialized staff, either in the library, broadly in their schools for the sciences, or directly within chemistry departments, to help their researchers meet the basic requirements imposed by funders. These staff can also advance the practice of data sharing by assisting chemists with some of the work required to deposit research data in online repositories. Institutions must also commit themselves to educating faculty members about how to responsibly manage data, and chemistry departments should foster discussion among their members about how and when research data should be shared.

Discovery Services

Problem statement: Chemists require highly customizable and efficient current awareness services.

The survey indicated that chemistry researchers are happy with the search tools that they have available to them; 73% of respondents reported that they are satisfied or very satisfied with the tools that they have for searching for chemistry literature. However, while researchers are happy with search tools, they do not always have good ways of keeping up with current research or efficiently browsing through newly-published papers for the serendipitous discovery of useful scholarship. Most of the interviewees reported a general anxiety about keeping up with the literature, and many chemists (including 58% of survey respondents) resort to inefficient techniques like skimming journals' table of contents to ensure that they have not missed any new information.

Recommendation

Although no service provider takes full organizational responsibility for discovery service provision, all providers (including libraries) have an opportunity to design discovery tools and services with better attention to the full needs of academic chemists. Such services will almost certainly require greater scale than any single university can provide, and so shared services or vended products will likely play a significant role in addressing chemists' need to maintain awareness of current scholarship. As these become available, libraries could move aggressively to help move chemists away from inefficient means of keeping up with current research, such as table of content alerts, and towards greater reliance on discovery services that better meet their needs.

Opportunity 1: Creating an alert system based on research interests

Chemists need a customizable alert service that can help them remain aware of the newest research in each of their core subfields without ignoring broader currents of relevance. In the survey, 57% of respondents said they would be likely to use such a service. Some providers already provide tools that alert them to new research, but not at the level of comprehensiveness and adaptability that chemists require. Ideally, its coverage would incorporate all journals in the field, as well as some supplemental materials such as patents, eTheses, and conference proceedings. It must be extremely timely, alerting against content at the point of publication or even beforehand. It must permit users to configure a set of core interests as well as a penumbra of broader secondary interests, against which alerting will trigger only for the very important materials. Such services will be most valuable if they can be targeted at the laboratory groups and collaborators and enable interactive peer-to-peer sharing.

Opportunity 2: Ensuring serendipity

Academic chemists rely on discipline-based conferences to expand their horizons and discover research that pulls their own work in new directions. Formal sessions, especially poster sessions, have real value in introducing chemists to new research in a highly digestible format. This type of discovery is enabled in part because chemists take time away from their day-to-day work to focus on learning about new research. While it may be difficult or impossible to replicate this kind of serendipitous discovery online, a service that provided brief opportunities to experience the work of other researchers without requiring travel could prove to be useful. There may be an opportunity to build a tool with a pricing model that provides an incentive for focused synchronous attention.

Opportunity 3: The review article

Review articles are vital discovery tools for chemists, even though, given the absence of original research, authoring one is assessed as a comparatively smaller scholarly contribution than authoring an original research article. In the survey, 66% of respondents said that review articles were an important means of learning about research, which ranked them above all other discovery mechanisms other than chemistry-specific journal search tools. Review articles have never been aggregated and integrated, nor have they been enhanced for the digital environment, but our research suggests that there may be opportunities to do so. A service that reframed the information from review articles as searchable networked bibliographies could prove incredibly valuable to chemists who are learning about new areas of research.

Research Dissemination Services

Problem statement: To navigate the complicated and in some cases apparently contradictory publication mandates from funders, institutions, and government, chemists require advisory services to support their research dissemination needs.

Our interviewees and the survey suggested that the majority of chemists are relatively uninterested in open access publishing, and many of them are relatively ill-informed about the major policy issues surrounding research publications and copyright. Many researchers feel that they have good access to all of the materials that they need, and they believe that almost everyone who needs access to their published papers can already do so. Chemists seek to have high impact in their field and to succeed in the Research Excellence Framework (REF). Even so, because of the Finch report and related initiatives, academia is adopting open access.

Recommendation

The nature of publishing research outputs is changing significantly as a result of new policies from funders and governments, and libraries have the opportunity to provide advisory and analytic services in support of these changes. The scenarios reviewed here need not be the exclusive province of the library, however, and funders, private companies, publishers, and others may be able to serve faculty members in these areas either independently or in partnership with campus libraries.

Opportunity 1: Publishing services center

The university, perhaps through its library, can provide advice and assistance on all of the steps in the publication process. Dedicated university staff should be available to help chemists review their obligations under funding agreements, identify channels to maximize their impact with key audiences, negotiate copyright agreements with potential publishers, and support them during the editing process. The library staff will also take responsibility for ensuring that publications are made available through online repositories whenever possible. In the survey, 48% of respondents said they would be likely to use the services of a publishing services center.

Opportunity 2: Research dissemination center

In this scenario, a campus-based center will take a broader role beyond publishing outputs to support all outputs that arise out of academic research, to include commercialization of research results through patents, start-ups, and other industrial partnerships. Chemists will work closely with the liaison staff of this research dissemination center at every stage of their research to ensure that new projects are designed and findings utilized to best effect. This research dissemination center would build on the valued services of universities' research offices, but also provide an "account management" model that ensures chemists have a single primary point of regular contact, or through an organizational model yet to be developed that incorporates both functions together.

Issues that Fall Out of Scope

In the course of our research, we encountered several issues that, while important, fall outside the intended scope of our project. For these, we feel it important to provide a problem statement but make no strong recommendations, hoping that others better positioned to consider these issues will do so. We would note that some of our recommendations above may be most effectively addressed by thinking holistically across many of the needs of academic chemists, including those identified here but held out of scope to the current project.

Laboratory management

Principal investigators lead research, but they also manage the work of their laboratory. This requires everything from budgeting and funding requests (which must integrate with other university offices) to goal-setting exercises (tied to the knowledge management described above) and chemical inventory management (which may connect to the university's environmental compliance office). Integrated laboratory management software that interoperates effectively with other university offices is not currently available, and as a result principal investigators experience a variety of unnecessary management challenges. This observation may help to inform the development of Research Management Services discussed above.

Accessing industrial funding

Many academic chemists have turned to a variety of industrial partnerships or funding arrangements to support their work. They often acquire these opportunities based on personal or idiosyncratic relationships. There are few if any systematic efforts at skills-building in how to generate these opportunities, and match-making services are not as well developed as they might be. This set of observations may help to inform the development of certain Research Dissemination Services discussed above.

Teaching Support Services

While this project did not directly address teaching services, several chemists indicated that they value their libraries in part for the assistance that they provide to undergraduates. Undergraduates use their campus libraries as a study space, they go there for materials like coursebooks, and in some cases they learn about the basic tenets of the bibliographic research process from reference librarians. There are many opportunities for libraries to expand and improve the services they provide to students, in many cases working in partnership with academic chemists.

Conclusion

Many types of research support providers, such as libraries, scholarly societies, discovery services, and software developers, can choose to make use of the scholar-centric findings and recommendations of this project in a variety of ways. It is perhaps worth emphasizing one core dynamic running through all of our recommendations. Each of the three services that we have identified and recommended would require a substantial reconfiguration, both in terms of the substance of the offering itself and the organization of its provision.

Some of these services would be expensive to implement; we have evaluated them based on their value to scholars, not on their cost. The question of whether they are worth the expense may depend on which organizations or providers choose to develop them.

The academic library was given special emphasis in this project. Today, based on the current array of service offerings, chemists value the library in their scholarly research only for its collections and little if at all for the services that it offers to add value elsewhere. In the service models recommended above, we see some real potential for the academic library to stretch the definition of the services it offers and its approach to offering value to the academic chemist. The library may also have a role in working with other service providers and ensuring that academics are aware of the latest research tools. It is clear from this project that libraries must think strategically about whether and how to invest in services for chemists.

Like academics in many other fields, chemists have real needs for a variety of research support services. Working creatively to address these needs should be a priority of all potential service providers.

Appendices

Appendix A: Interview Protocols

Service Providers Interview Guide

Current services provided

- What support services are currently being provided to chemistry faculty?
- Which services are new in the past three years, or are under development?
- What is your mission/strategy/goal for providing support services to chemistry scholars?
- How do you evaluate the effectiveness or success of your current services?
- How do these support services fit in with the broader landscape of the support available to chemists?

Planning for future services

- Looking forward, what types of expanded support are you hoping to provide for chemistry faculty?
- What do you need in order to support chemists effectively?
- How do you decide which new services to offer and which to retire?

Challenges

- What challenges do service providers face in supporting evolving faculty research practices?

Faculty interview Guide

Warm-up

- Thinking back to your PhD work and your post-graduate lab work, how would you describe your training as a chemist?
- Tell me about the research you did as a graduate student.
- How does the work you do today differ from your work as a graduate student?
  - How is it more efficient?
  - How is it more challenging?

Current research

What research methodologies (not including experiments) are currently in use and how are these expected to change?
What support is available – locally or distributed – to help facilitate the research process?
How do chemists approach their research and use scholarly publications?
How are chemists tracking citations and publications?

- Research topic
  - Tell me about a research project you're working on right now.
  - When was this project first conceived?
  - Is this a continuation of previous research or a new area for you?
  - How did you decide to pursue this project?
  - What do you do when you're pursuing a new project/topic? Where do you start?
- Funding
  - Did you pursue funding for this project? Tell me about that process.
- Research notes management
  - How do you keep track of the articles, images, data you've gathered for this project?
  - How do you keep track of the data, articles, etc. that you're producing as part of this project?
- Collaboration
  - Are you working with others at your institution? From another institution? From another country?
  - Tell me more about the nature of your collaborative relationship.
    - Is there a clear delineation of responsibilities? Are you partners at every step?
    - How's it going? Challenges?
    - What tools help you collaborate more effectively?
- Challenges
  - What is going really well with your project?
  - What obstacles have you experienced so far?

Discovery

What networks do chemists use to gather their research materials?

- Tell me about the desk research you've been doing for this project – outside of lab experiments.
- What resources are you using? To what extent are you interested in published articles (and other descriptions of experiments etc) vs. reviews vs. databases of compounds etc? In other words, what exactly do you need as inputs to support your research vs. citations to support your publication of that research?
- How do you keep up with literature in the field?
- How do you locate data? What type of data are you looking for/using?
- What are your go-to tools, websites, publications?
- What challenges have you had recently when looking for literature or data?
- What do you do when you can't find something?

In the lab

How are chemists managing the work of their labs?

- Tell me about how your lab works.
- How do you share, organize, save, research notes within your group?
- What happens to lab notebooks when students leave your lab?
- Do you use ELNS?
- What challenges is your lab facing in managing work/information collaboratively?

Library and resources

How are chemists using the library?
What do chemists want from the library, both immediately, and in the long term?
Are library collections are meeting chemists research needs?

- Tell me about the last time you were looking for an article.
- What tools did you use to find the information you needed?
- How do you organize your research literature? At the lab level?
- At what points in your research process do you turn to the literature? Do you look up reactions, etc..?
- Tell me about the last time you went to the library.
- How would you describe the role of the library in your research?
- Were all the resources you needed for this project available on campus? Articles? Data?
- When was the last time you spoke to a librarian? Tell me about that conversation.
- Did the librarian add value? In what way?
- If not, do you understand what the librarian's role is and why he/she is there?
- Do you value him/her even if you don't engage directly? Why?
- What would you like librarians to do that they do not currently?
- What databases do you use regularly?
- What other online resources are critical to your research?
- What obstacles have you encountered when using the library?

Data management

How are chemists managing and publishing/distributing the research data they produce? Learning how chemists are using data, what types of data they are producing and acquiring, and what they need to support their work with data

- What types of data are you producing?
- Where do you keep it? How long do you keep it for?
- What data do you submit for publication?
- Have you ever sent a data set to a colleague? Or requested one from a colleague? (For a collaborative project, or otherwise.)
- Have you ever deposited data in a repository?
  - What was your motivation for depositing? You were required? For preservation? For sharing?
  - Was OA an important motivator for depositing? Why?
- Have you ever used someone else's data from a repository?
- Have you ever found it useful to have access to your own data through a repository?
- Which repositories?
- How do you feel about making data OA?
- What challenges are you having in managing the data your group/research teams?

Publishing

How are chemists publishing their research?

- Tell me about the last time you published an article?
  - Why was it important to you or to the audience for your research that you format your research findings as an article?
  - What happened to the data set that accompanied the article?
  - How do you store your data?
  - Who did you publish with? How long did review take?
- Open access
  - Have you ever made an article available open access?
- Collaboration
  - Tell me about the role of collaboration and co-authoring in your publication process.
  - How do you share files and drafts and data between authors?
- Thinking about the publication processes – what challenges are you facing? Is your lab team facing?

Future

- Looking forward, what challenges do you see for yourself as you continue to do research?

- Challenges for the field?

- What does the field need to move forward effectively?

Wrap-up

- Looking back on our conversation today, can you reflect on how your research practices have changed or are changing?

- What's exciting that happening in the field right now?

- If I gave you a magic wand that could help you with your research and publication process – what would you ask it to do?
  - What do you wish the library could do for you?
  - What do you wish the university could do for you?
  - What do you wish shared services could do to address cross-institutional needs?

Appendix B: Interviewees[12]

Phillip Adler
Graduate Student,
University of Southampton

Perdita Barron
Reader in Biophysical Chemistry,
University of Edinburgh

Mike Bearpark
Reader in Computational Chemistry,
Imperial College

Martin Beeson
Queen Mary University London Library,
Senior Academic Liaison Librarian (Science and Engineering)

Lisa Blair
University of South Hampton

Lee Brammer
Professor of Inorganic and Solid State
Chemistry, University of Sheffield

Neil Bricklebank
Senior Lecturer in Inorganic Chemistry,
Sheffield Hallam University

Matthew Clough
Research Postgraduate, Imperial College

Matthew Davidson
Bath PhD Training Center,
Professor of Inorganic Chemistry

Iain Day
Lecturer in Chemistry and NMR
Spectroscopy, University of Sussex

Graeme Day
Royal Society University Research Fellow,
University of Cambridge

Martin Dove
Professor and Director of the Centre for
Condensed Matter and Materials Physics,
Queen Mary University of London

Karen Edler
Reader in Physical Chemistry,
University of Bath

Thomas Faust
Doctoral Prize Fellow,
University of Manchester

Andrew Fogg
Royal Society University Research Fellow,
Liverpool University

Stephen Goldup
Royal Society University Research Fellow,
Queen Mary University of London

Jonathan Goodman
Reader in Chemistry,
University of Cambridge

Nick Greeves
Senior Lecturer, University of Liverpool

Neil Grindley
JISC, Programme Manager, Digital
Infrastructure (Digital Preservation)

Simon Higgins
Reader in Chemistry,
University of Liverpool

Mike Hill
University of Bath, Professor of Inorganic
Chemistry; Royal Society of Chemistry
Dalton Division Council, Treasurer

Simon Hodson
JISC, Programme Manager, Digital
Infrastructure, Managing Research Data

Linda Humphreys
Bath, Library, Science Faculty Librarian

Richard Jackson
Professor of Synthetic Organic Chemistry,
University of Sheffield

Kara Jones
Bath Library,
Research Publication Librarian

Nazira Karokia
Associate Dean and Senior Lecturer,
Bradford University

Alex Lawrenson
Liverpool University

Richard Layfield
Lecturer in Inorganic Chemistry,
University of Manchester

Mark Light
X-Ray Diffraction Manager,
University of Southampton

Jason Loader
Graduate Student, University of Sheffield

Liz Lyon
Bath, UKOLN,
Digital Curation Center, Director

12 The interviewees' titles and institutional affiliations as listed here reflect their positions at the time of their interviews for this project.

Johanna McEntyre
UKPMC, Head of Literature and Services at EMBL-EBI

Leah Rae McEwen
Cornell University Library, Associate Librarian

Lynne Meehan
UCL Library, Science Subject Librarian

Bao Nguyen
Ramsay Memorial Fellow, Imperial College

Claire Packham
British Library-Sciences, Science Reference Team Leader

Jiayun Pang
Senior Lecturer in Computational Chemistry, Greenwich University

Dan Pantos
Lecturer, University of Bath

Don Parkin
Chemical Database Service, Chemical Database Manager at STFC

Dixit Parmar
Graduate Student, University of Manchester

Simon Parsons
Professor of Crystallography, University of Edinburgh

Justin Perry
University Enterprise Fellow, Northumbria University

Andy Platt
Senior Lecturer in Forensic Science, Staffordshire University

Alena Ptak-Danchak
Oxford Library, Head of Science and Medical Libraries

Robert Raja
Reader in Chemistry, University of South Hampton

Ljilja Ristic
Oxford Library, Physical Sciences Librarian & Subject Specialist

Ellie Roberts
Surrey Library, Academic Liaison Librarian, Faculty of Health and Medical Sciences

Peggy Schaeffer
Dryad Repository: Biosciences, UNC Chapel Hill, Communications Coordinator

Eugen Stulz
Senior Lecturer in Bio-organic and Materials Chemistry, University of South Hampton

Martin Sweet
EPSRC, Portfolio Manager

Katherine Thompson
Imperial College Library, Liaison Librarian: Natural Sciences

Bruce Turnbull
University of Leeds, Royal Society Fellow; Royal Society of Chemistry Carbohydrate Committee, Secretary

Michelle Walker
Northumbria Library, Library Liaison Advisor

Tom Welton
Head of Department and Professor of Sustainable Chemistry, Imperial College

Richard Whitby
Dial a Molecule, Southampton, Professor and Dial-a-Molecule Network Coordinator

Anthony Williams
Royal Society of Chemistry, ChemSpider, Vice-President of Strategic Development

James Wilton- Ely
Lecturer in Inorganic Chemistry, Imperial College