# Identifying the Knowledge and Skills that Doctoral Chemists Require in the Workplace

by

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A dissertation submitted to the Graduate Faculty of
Auburn University
in partial fulfillment of the
requirements for the Degree of
Doctor of Philosophy

Auburn, Alabama
May 1, 2021

Keywords: Chemical Education Research, Graduate Education/Research, Qualitative Analysis, Quantitative Analysis, Professional Development



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## Abstract

In 2012, the National Research Council and the American Chemical Society reported many critiques of graduate education in the chemical sciences that do not adequately prepare students for the interdisciplinary careers for which they are training. These reports highlight the need for graduate students to possess knowledge and skills necessary to perform in careers as chemists in academia, industry, and other sectors. Despite abundant suggestions and recommendations, very few efforts have been made to evaluate and assess what knowledge and skills the chemists possess in their current work. The new investigation here expands on the previous work by identifying the knowledge and skills required for careers in the academic and non-academic chemical sciences. To achieve this goal, a total of 31 doctoral chemists from academia, industry, and government were interviewed about the activities they conduct on a day-to-day basis and the knowledge and skills that were required to complete these activities. In this qualitative study, there were 12 major knowledge and skills identified by thematic analysis, such as communication skills, management skills, teaching skills. Based on the results, a quantitative instrument was developed and piloted amongst 60 chemists. Various sources of evidence were gathered to demonstrate the validity and reliability of the online survey. After validation, the full survey was distributed with the aim of achieving a national level picture of the knowledge and skills that were required by doctoral chemists in different job sectors. A total of 412 responses were collected and analyzed by descriptive and inferential statistics to indicate differences that exist in the knowledge and skills between the different job sectors.

## Acknowledgments

The journey has been utterly hard and life-changing at the same time. Thank my advisor, Dr. Jordan Harshman. I am incredibly grateful to have been supported and cheered on by such a wonderful mentor. I am deeply honored to have been under his guidance. Thank all the group members, Dr. Brittany Busby, Tingting Qu, they give me research suggestions and emotional support. Thank Mercedes for working on virtual reality chemistry laboratory tutorial project with me. Thank Emily and Yousif for their support on my research. Thank Auburn University and the Department of Chemistry and Biochemistry. Thank all the committee members and university reader for spending their valuable time on my research, oral exam, annual report and dissertation. Thank all the participants and collaborators, they all have a big interest in helping graduate students make successful transition into a job, we do appreciate their time and contributions. Thank my parents and many of my friends, they care about me and give me support at all times.

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## List of Abbreviations

| | |
|---|---|
| ACS | American Chemical Society |
| B.S. | Bachelor of Science |
| Ph.D. | Doctor of Philosophy |
| R&D | Research & Development |
| IRB | Institutional Review Board |
| IRR | Inter-Rater Reliability |
| AERA | American Educational Research Association |
| APA | American Psychological Association |
| NCME | National Council on Measurement in Education |
| ANOVA | Analysis of Variance |
| TA | Teaching Assistant |
| EFA | Exploratory Factor Analysis |
| CFA | Confirmatory Factor Analysis |
| MANOVA | Multivariate analysis of variance |
| NSF | National Science Foundation |
| VSEPR | Valence Shell Electron Pair Repulsion Theory |
| CHIRAL | Chemistry Instrument Review and Assessment Library |
| STEM | Science, Technology, Engineering, and Math |

In this dissertation, Chapter 1 describes the background of this project, research questions posed to be addressed, and theoretical frameworks used in this study. Chapter 2 includes the research methods employed for qualitative study, survey development, and quantitative full study. Chapter 3 provides the results and discussions of qualitative study, survey development, and quantitative full study. Chapter 4 summarized the key findings obtained from this project, the limitations, and the implications for researchers and educators.

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Next, a follow-up study looking at the daily experiences of doctoral chemists was included in Chapter 5. This is a side project regarding graduate education, but it is not directly related to the primary research questions in this dissertation. Chapter 6 and Chapter 7 are side projects dealing with undergraduate education.

# CHAPTER 1: INTRODUCTION

Chemistry doctoral education has played a critical role in the success of the U.S. workforce and economy by providing the knowledge and skills that future scientists need to solve the world's largest issues. In 2012, the National Research Council[1] and the American Chemical Society[2] highlighted the need for graduate students to acquire the necessary knowledge and skills to perform in careers as chemists, but they also reported many criticisms that doctoral programs in chemistry do not adequately prepare their students for future chemistry careers. These criticisms, which have persisted since the late '40s [3–7] (ACS reports from the Committee on Professional Training), claim that doctoral students are over-specialized, lack interdisciplinary experiences, and are trained poorly for non-academic sectors. While a rather bleak picture of doctoral training in chemistry (and other sciences[8]) is presented in the literature, society has reaped benefits of the advanced training that chemists have received in their doctoral programs in the form of technology and products. The goal of the present study is to examine the knowledge and skills that chemists use in typical chemistry careers. This information can be used to illuminate learning targets for doctoral programs in chemistry, potentially revealing knowledge and skills that are vital for success in chemistry careers, but perhaps under-emphasized in doctoral programs.

## Previously identified criticisms of chemistry graduate education

Doctoral chemistry graduate students have a variety of career paths that they can take as chemists in the academic, industrial, governmental, and other sectors. The majority of chemists end up with industrial positions immediately following their doctoral education,[9] a fact reflected in current population estimates of chemists (**Table 1**).[10] Of the percentage in academia, there are few details for how many occupy primarily research, primarily teaching, or temporary postdoctoral positions, but a good mix can be expected given the distribution of schools across the Carnegie Classifications[11]. It is surprising, therefore, that chemistry graduate programs often focus on training doctoral students for careers in research-intensive, academic positions as the relative minority of students will end up in these careers.[1,2] This potential misalignment of training and career has led to lower satisfaction levels in the professional training doctoral students receive in graduate school.[2]

In a survey of approximately 2,300 chemistry graduate students[12], the ACS reported that only a quarter of them felt they were provided with information about non-academic career paths and over 40% did not feel that their advisors supported their choices of career paths. At the same time, chemists in academia, industry, and government claim that graduate students are not adequately prepared for current and future careers, a sentiment echoed in multiple national reports regarding graduate education in the physical sciences over the past couple decades.[8,13–18] Industrial members report dissatisfaction with the lack of knowledge to distinguish between academic and non-academic cultures, suggesting that this industrial sector requires more non-technical skills than other sectors, but details about which skills and what they entail are sparse.

**Table 1. Distribution of Chemists in Broad Sectors**

| Sector | National Distribution (%)[a] |
|---|---|
| Academia | 37 – 50 |
| Industry | 43 – 56 |
| Government | 6 – 7 |
| [a]See refs 9 and 10. | |

Chemists who work in industry or government have anecdotally reported that their employees require skills and knowledge not traditionally taught in graduate school.[2] In particular, teaching[2,19], safety[2,20], and so-called "soft skills" (i.e. communication, teamwork, etc.)[21,22] are commonly reported as inadequate, leading to expensive retraining periods for new employees and issues in employee retention[2]. A solution from ACS has included inviting chemists from all sectors into to discuss what skills are necessary for each sector.[23–27] These conferences have identified some skills such as communication and teamwork, but do not reach these conclusions on the basis of empirical research. Because a graduate degree is the only path that allows the technical training required for all sectors of chemistry, chemistry departments are responsible for identifying the knowledge and skills that are aligned with the American workforce needs and making chemists successful in their careers. In addition to anecdotal perspectives that are valuable for discussion, empirical research is warranted to identify the knowledge and skills required for chemists.

Research into the necessary knowledge and skills that undergraduate students need to secure and to be successful in jobs is abundant.[28–30] Despite significant differences in educational systems and job markets at the undergraduate and graduate levels, studies from several countries[31-33] point to a key set of knowledge and skills that (B.S.) graduates will need to obtain. However, these students are not generally specific to the job market and culture of chemistry. Instead, they report employers' expectations across all science and humanities fields. Additionally, while some overlap in requisite knowledge and skills between a bachelor and doctoral chemist is expected, jobs that require a Ph.D. versus a bachelor are clearly looking for a different set of knowledge and skills. This raises a serious question of how applicable the findings of studies that mostly focus on employer expectations of the undergraduate population are to doctoral students.[22] Finally, even under the assumption that undergraduate, domain nonspecific skills are applicable to doctoral chemists, much of the knowledge and skills reported in previous literature are not well-defined.[34] For example, reports have ubiquitously stressed the importance of "written communication skills", but do not explain what is meant by this term. We can postulate that "written communication skills" can mean very different things to a research-intensive professor and an industrial R&D chemist. A lack of well-defined knowledge and skills lead to ambiguity of what is truly required for various positions in chemistry.

Most faculty members do not have significant experiences outside of academia and therefore may not be able to identify the specific knowledge and skills required for other career paths. Without systematic research to identify these knowledge and skills required by doctoral chemists, faculty in chemistry departments design their programs with the knowledge and skills that they believe will be necessary for chemistry careers. However, if the knowledge and skills required by typical positions in chemistry can be clearly identified and implemented, faculty can design their doctoral programs to help graduate students develop those skills.

**Research questions**

With the need to identify the knowledge and skills that U.S. chemists with doctoral degrees require to be successful in their jobs, our present goal is to minimize the uncertainty in identifying rich and rigorous descriptions of the knowledge and skills that are required by typical careers in chemical sciences. In doing so, we pose the following research questions:

*RQ1: What knowledge and skills do doctoral chemists in different job sectors perceive to be necessary for their careers?*

*RQ2: How does job sector affect the way that chemists require and/or value certain knowledge and skills over other sectors?*

**Theoretical framework**

The goal of this study aligns with the theories of socialization and cognitive apprenticeship. Scientists engage in socialization as they develop knowledge and skills and teach new-coming chemists.[35] Socialization is described as the process of obtaining the advanced knowledge and skills that are required for a certain career. There are four stages in socialization: anticipatory (being aware of new roles and procedures), formal (observing and learning these roles through formal training), informal (observing and learning these roles through informal interactions), and personal (fusion of roles with individual values). [36] In this project, it was therefore important to measure knowledge and skills specifically within the context of participants' everyday activities (as opposed to abstract the knowledge and skills a chemist needs in general). We also used this theory to abstract knowledge and skills from descriptions of the activities in which chemists partake on a daily basis.

The cognitive apprenticeship model was proposed to describe the transfer of knowledge and skills from expert to novice. In the literature, cognitive apprenticeship has been a long-accepted model of graduate education.[5, 37-39] According to the model, novice (graduate student) and expert (advisor) go through modeling, coaching, scaffolding, articulation & reflecting, and promoting transfer of learning stages.[40] The key aspect of the cognitive apprenticeship approach is that knowledge and skills gained by trainees are situated within a context. This means that learning does not occur isolated from context but occurs for a specific purpose, vocation, or within a certain culture. Therefore, graduate schools' responsibility in preparing students for a wide variety of careers in chemistry will be best served through a better understanding of the knowledge and skills required in many of these and other job sectors.

# CHAPTER 2: METHODS

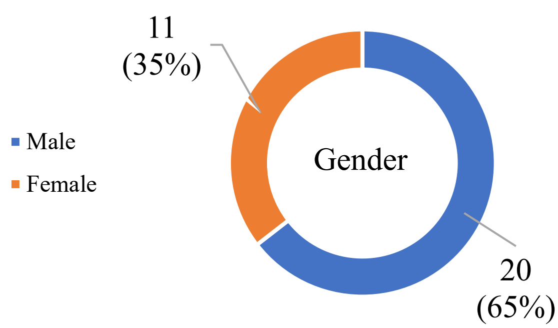
## Research methods employed-Qualitative study

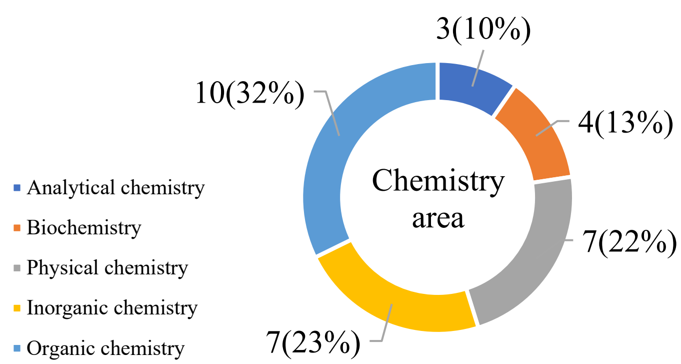
### Participants and settings

With the goal of identifying knowledge and skills that chemists require, it was important to sample purposefully among chemists in academia (research-intensive and teaching-intensive), government, and industry (different industrial positions). The participants of the study were required to hold a doctorate in chemistry and have careers in chemical sciences. The contact information of 700 faculty from 77 academic institutions was collected from departmental websites. The first author selected 30 faculty from 30 institutions from this list at random each day. A total of 410 faculty were invited, and 15 of them participated in this study. Contact information for industrial and government chemists was not readily available online, so we relied on snowball sampling41 to identify potential participants after recruiting initial chemists within the networks of our colleagues. Initial participants then invited others inside and outside of their companies to participate in this project. We purposefully invited chemists from large and small companies as well as a variety of position types in an attempt to achieve a broad distribution of chemists.

A total of 31 chemists (20 males and 11 females) participated in this study (**Figure 1**). The sample covered a variety of disciplines within chemistry. Fifteen unique academic institutions were represented in this study, one per each of the 15 faculty members in the sample. Of the research faculty, 22%, 22%, and 56% were assistant, associate, and full professors, respectively. And of the teaching faculty, 50% of each were associate professors and lecturers, respectively. All nine research faculty took on teaching as their secondary position, while only one teaching faculty took on additional research work beyond the primary duty.

**Figure 1. Background Information of Participants**




Nine unique companies were represented across 14 industrial chemists, seven of which were large companies with over 500 employees and two of which were smaller companies with fewer than 500 employees. Industrial chemists self-categorized their work responsibilities as research & development (R&D), management and consultant (see **Table 2**). Of the 14 industrial chemists, 12 held primary positions in R&D and two worked primarily in management positions. Additionally, two government scientists from two different state agencies also participated in the study. The primary job responsibility for both scientists was R&D, and management was their secondary responsibility. The goal of the sampling method was not to interview multiple people from each specific career that a chemist occupied as chemists can occupy hundreds of specific careers. Instead, we sought to gain the perspective of the most common jobs that chemists take on to have a maximum impact. As referenced earlier, slightly less than half of the chemists will have a primary work function involving teaching and/or research in academic institutions. Industry also represents about half of all chemists and 76% of these chemists fall into either R&D or management as their primary work function[10]. Thus, this study focuses on chemists who do R&D, management, research, and teaching as their primary work function(s), because more than 80% of all chemists share these work functions.

**Table 2. Summary of Participants by Sector and Work Function**

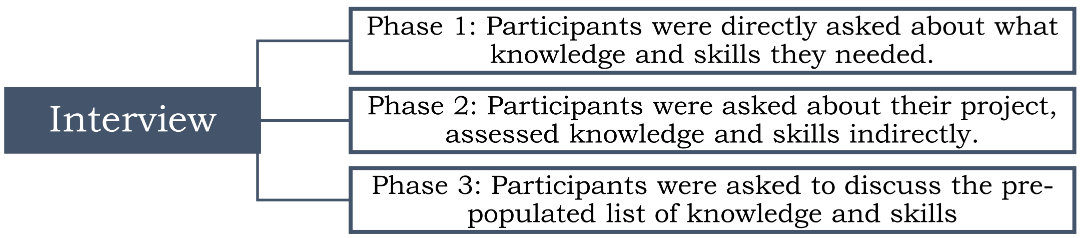
| Job Sector | Work Function Responsibility | | Total Participants, $N$=31 | | |
|---|---|---|---|---|---|
| | Primary | Secondary | $N$ | % | Subgroups |
| Academia | Teaching | - | 5 | 16 | $N_1 = 15$ |
| | Teaching | Research | 1 | 3 | |
| | Research | Teaching | 9 | 29 | |
| Industry | R & D | - | 8 | 26 | $N_2 = 14$ |
| | R & D | Management | 3 | 10 | |
| | R & D | Consultant | 1 | 3 | |
| | Management | - | 2 | 6 | |
| Government | R & D | Management | 2 | 6 | $N_3 = 2$ |

**Data collection**

All chemists were invited via email to participate in semi-structured interviews[41] conducted electronically and recorded with the permission of participants according to IRB regulations (#17-362, Auburn University). The semi-structured interview approach was used to explore individual experiences and perceptions[41]. The research was conducted ethically with informed consent of the participants.

In order to directly and indirectly identify and explore the knowledge and skills that doctoral chemists require, a 3-phase interview protocol was designed (**Figure 2**). The participants were first asked for a brief description of their position, the activities they conduct on a day-to-day basis, and what knowledge and skills were required to do their jobs (Phase 1). After each response, follow-up questions were asked to elicit how that chemist understood the particular knowledge or skill by breaking it into smaller knowledge and skills and providing examples. Because it has been reported that non-technical skills are under-emphasized in graduate school2 and details about what these skills entail are sparse, the follow-up questions were asked to focus on “soft skills” instead of looking for specific chemistry knowledge. Thus, in Phase 1 participants were directly asked about what knowledge and skills they needed to successfully conduct their job. In Phase 2, participants were asked to describe a project that they had been recently working on and how they overcame challenges during their work. This phase indirectly assessed knowledge and skills and allowed the abstraction of them from the participants’ descriptions. In Phase 3, a list of knowledge and skills was gathered from the most commonly discussed skills in previously reported literature[21,22,24,28,29,32,34,38], surveys[6,7,14,31,33], and national reports[1,2,17,18]. Participants were presented with this pre-populated list of knowledge and skills that chemists may require for their jobs, and they were asked for general (dis)agreement (without explicitly rating them). This final phase was designed to ensure that chemists had the opportunity to discuss knowledge and skills they may not have brought up in Phase 1 & 2, but were asked last so as not to influence their original thoughts. We did not gather enough evidence to suggest that participants' responses in this phase reflected their genuine thoughts. Rather, responses were generally shallow and likely influenced by social pressure to respond positively to most knowledge and skills. Therefore, responses to this section represent a vast minority of the development of themes and most coding occurred in the first two portions of the interviews. The full protocol can be found in Appendix 1 in the Supporting Information.

**Figure 2. Interview Phases**




**Data analysis**

All interviews were transcribed verbatim (See Appendix 4 for three example transcripts), and thematic analysis[41] of the 31 transcripts was conducted using the qualitative data analysis software Dedoose through a multistage coding process. Thematic analysis can be used to identify the detailed information behind codes and understand how key factors influence success in the common chemistry workplace. The first step of coding involved reviewing the interview transcripts thoroughly and highlighting salient features of the data related to the research questions and providing that data with a code. Next, a list of codes was compared and sorted into categories. Then, the authors synthesized those categories which were similar in nature and derived themes depending on how they related to the research questions.

Three inter-rater reliability (IRR) metrics are displayed in **Table 3** to demonstrate the trustworthiness of data. Three coders applied codes independently for a set of subjects to compare the co-occurrence of coding across 21% of all codes. Percent agreement is the most commonly used statistic to compute IRR, but this seemingly simple statistic can be computed in many different ways, leading to more conservative (lower values than expected) or more liberal estimates (higher values than expected)[42]. For our project, if one coder among three coders disagreed with the other two on a specific code, the agreement was calculated as 50%, which is the average of 67% (assume the majority coded correctly) and 33% (assume the minority coded correctly). The average of the conservative and liberal agreement indices was calculated, resulting in 85.8% agreement. Fleiss' kappa[43] aligned with Krippendorff's alpha[44], which both indicated acceptable IRR[45] (See Appendix 2 for code).

**Table 3. Inter-Rater Reliability Results**

| Inter-Rater Reliability Methods | Results |
|---|---|
| Agreement,[a] % | 0.86 |
| Fleiss's K Value,[b] | 0.80 |
| Krippendorff's α Value,[b] | 0.80 |

[a]If one coder among three disagreed on a code, the agreement was calculated as 50% (avg. of 67% [majority correct] and 33% [minority correct]). The average of the conservative and liberal agreement indices was calculated, resulting in 85.8% agreement. [b]Fleiss's K aligned with Krippendorff's α; both indicated acceptable IRR. See the Supporting Information, Appendix 2, for code.

**Research methods employed -Survey development**

The study includes three stages: (1) use the qualitative results to develop items of doctoral chemists' knowledge and skills for a quantitative instrument, (2) a pilot study of this instrument and instrument modification, and (3) gathering of validity and reliability evidence for the modified instrument. The details for each stage will be outlined separately in the subsequent sections.

**Survey development**

A well-designed survey should meet the research objectives mentioned in chapter 1, should be well-organized and worded to encourage participants to respond with accurate and unbiased information, and should be well-arranged so that the participants remain interested throughout the survey[50].

The survey items derived from the results of the previously discussed qualitative study and literature. This scale asks participants to mark their agreement to each statement that complete the following phrase:

*In order to do my job successfully, it is necessary to...*

The stem landed on measuring perceptions of knowledge and skills needed for success in doctoral chemists' jobs in order to meet the survey's objectives, which is about identifying the knowledge and skills that chemists require for their careers. Additionally, this survey intended to measure the necessity of the knowledge and skills, but not the frequency used by each participant. It was corresponded to the research questions and avoided introducing frequency bias into the data.

The responses to this stem include 73 items to measure the knowledge and skills that doctoral chemists perceive to be necessary for their careers. Sample items include ''build and develop professional relationships inside my organization'' and ''work with people with different roles and responsibilities in a group to pursue common goals''.

A six-point Likert scale and a separate option of *Not Applicable* were used, with 1 for ‘‘*Strongly Disagree*’’, 2 for “*Disagree*”, 3 for ‘‘*Somewhat Disagree*’’, 4 for ‘‘*Somewhat Agree*’’, 5 for “*Agree*”, 6 for ‘‘*Strongly Agree*’’, and 0 for “*Not Applicable*”. Please see Appendix 6 for all items.

A person's attention may change during the survey, in order to avoid careless responses or errors, a total of two focus check questions were designed in the survey. When analyzing the data, only observations with correct responses for both focus check questions were kept for further data analysis.

The survey was expected to be finished within 15 minutes to complete the 73 items and demographics form. To ameliorate stereotype threat[76], the demographic items were placed at the end of the survey starting from a separate page. The demographic item formats included multiple choice for types of job sectors (three categories plus a free response option), gender (three categories plus a free response option), race/ethnicity (six categories plus a free response option).

**Pilot study**

In order to determine whether the survey is well-designed and going to achieve the desired results, it is necessary to pre-test the questionnaire before using a full-scale survey. This developed survey was piloted with 60 respondents to identify any mistakes with wording and other potential problems that need to be corrected. Those participants were asked to check the issue box if they found there was any issue with understanding of the item. The assessments were conducted to verify that the resulting values represent credible evidence. This instrument was in line with the approach to test validity in standardized tests, which suggested that possible mismatches between intended and actual measurements should be revised or eliminated.

Subsequently, the pilot participants were also invited to complete a brief validation interview (less than 30 minutes) to assess readability. Items were reviewed in the interview on the basis of whether they were clear and to what extent the response options aligned with their beliefs. Items with wording issues were either rewritten or eliminated from the survey list. Additionally, the participants were asked to take the survey again to determine test-retest reliability.

The data were not sensitive in nature and accidental disclosure would not place the participants at risk; no identifiers linked individuals to their responses. Consent to use the survey data was gathered using a cover page on the survey, clearly stating that participation in the study was voluntary and anonymous.

**Participants**

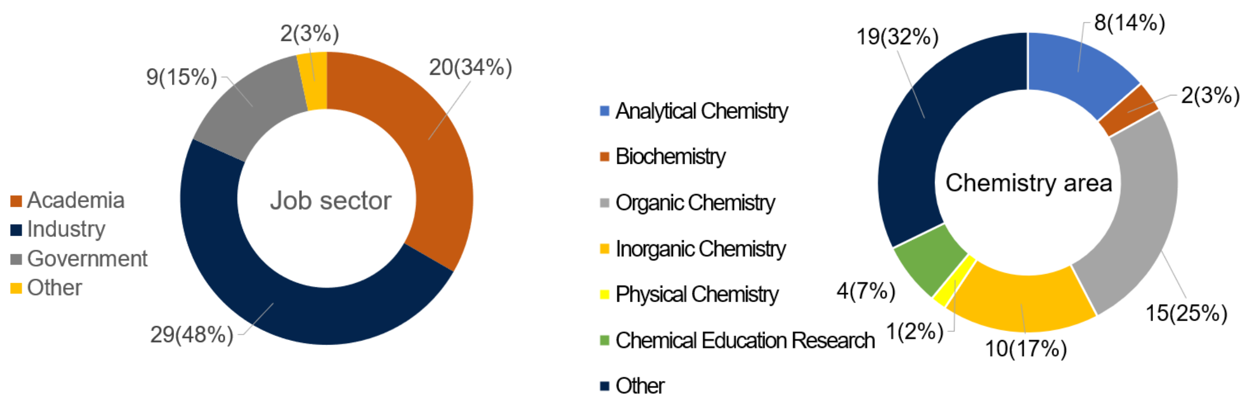
In stage 2, the participants of the study were required to hold a doctorate in chemistry and have careers in chemical sciences. Additionally, the respondents selected for the pilot survey were broadly representative of the different types of chemists in various positions. It was important to sample purposefully among chemists in academia (research intensive), academia (teaching intensive), government, industrial, and other positions.

Contact information for faculty was readily found by scraping departmental websites, a total of 5450 faculty members from 207 institutions were collected in a master list. Faculty members from different types of institutions were purposefully selected for pilot study. The institutions included 2-year college, community college, 4-year liberal arts college, 4-year comprehensive college, and 4-year research college.

Industrial and government chemists were not commonly available online. After identifying several participants, purposeful and snowball sampling[21] were used to identify potential participants from industry and government. Representatives from a list of companies and participants of the qualitative study were contacted with a letter of our research aim and the request of distributing the invitation to their colleagues and collaborators by snowball sampling. The purposeful sample was designed to invite chemists from a variety of position types. These potential participants were found through personal networks of our colleagues.

A total of 61 doctoral chemists took this survey ("Time 1"). After checking for missing data and careless responses (e.g., the same response for all the questions), one response was deleted (the participant had wrong responses for both focus check questions), which yielded 60 participants with usable data. Of the 60 participants, 66.7% were males, 31.7% were females, and 1.7% were unknown. In **Figure 3**, 33.7% were from academia, 48.3% were from industry, 15.1% were from government and 3.3% were from other job sectors. The sample covered a variety of areas within chemistry.

**Figure 3. Participants' Background Information in Pilot Study**




During stage 3, qualitative and quantitative approaches were used to gather evidence for validity and reliability of the online survey.

***Interview participants***

In stage 3, doctoral chemists were recruited from the list of chemists that completed the first survey. Interview participants were invited at the end of the survey. In accordance with Institutional Review Board policy, participants were informed that their participation was confidential and that they would be volunteering for a research study regarding their perceptions of the design of the online survey. Interested chemists volunteered by typing their name and email address to a redirected link. Volunteers were contacted via email to arrange a less than 30-minute interview time slot. A total of 19 participants were interviewed, the interview protocol was approved by the Institutional Review Board. Of the 19 participants, 47.3% were from academia, 42.1% were from industry, 10.5% were from government.

***Retest participants***

In stage 3, the questionnaire was administered again to assess the test-retest reliability. Participants that completed the first survey ("Time 1") were invited to take the survey again ("Time 2") two weeks after "Time 1". "Time 1" data was used to investigate internal structure, and both ''Time 1'' and ''Time 2" data were used for test-retest reliability. At Time 2, 12 participants took the same survey two weeks after they completed the first one. For these 12 chemists, 50% were male, 50% were female. 58.3% were from academia, 33.3% were from industry, 8.3% were from government.

A $10 Amazon gift card was given if participants took the survey and follow-up validation interview; a $20 Amazon gift card was given if participants took the survey twice as well as follow-up interview. In addition, there was 1:500 chance to win $100 for all participants.

Based on the available demographic information, chemists who responded to the survey at Time 1 and chemists who participated in validation interview can roughly represent the national distribution of chemists in broad job sectors. Chemists who responded to the survey at Time 2 were slightly more representative of academia (**Table 4**).

**Table 4. Participants Distribution in Pilot Study**

| | Time 1 $N_1 = 60$ | Validation interview $N_2 = 19$ | Time 2 $N_3 = 12$ |
|---|---|---|---|
| Academia | 20 (33.3%) | 9 (47.3%) | 7 (58.3%) |
| Industry | 29 (48.3%) | 8 (42.1%) | 4 (33.3%) |
| Other | 11 (18.3%) | 2 (10.5%) | 1 (8.3%) |

**Interview protocol**

All validation interviews took place via Zoom to ensure both participant confidentiality and audio / video quality. Prior to the interview, participants were asked to complete the survey and marked issues when they were taking this questionnaire. Upon completion of the instrument, the participants who were interested in the validation interview were contacted via email. In the interview, participants were asked to think aloud and explain their reasoning of the choices they made for some items and their understanding of the issue items that they marked. If a participant's understanding of the item did not match the survey's intention, probing questions were asked in order to clarify their interpretation of the items. This methodology is important in establishing evidence for the response process validity[77] of an instrument, ensuring proper readability, and consistency between participants' understanding among the target population[78]. In addition to asking probing questions regarding a single item and its interpretation, suggestions of adding additional knowledge and skills were sought in the interviews. Furthermore, whether the use of a Likert-type scale was appropriate was explored. The full protocol can be found in Appendix 5.

**Instrument modification**

The instrument measures the knowledge and skills that doctoral chemists perceive to be necessary for their careers, which can complete the phrase:

*In order to do my job successfully, it is necessary to...*

Evidence based on test content was gathered by having an expert panel, comprised of four chemistry education researchers. The first round of modification was made by discussing the level of representativity and exhaustiveness of survey items. After conducting validation interview, evidence based on response process was collected. A total of 72 items were retained from the original 73-item survey with one modification based on the responses of interviews. The six-point-Likert scale and *Not Applicable* option were kept. The exploratory factor analysis was then adopted to search for the structure among the set of knowledge and skills, and therefore, the results indicated if further revisions were needed.

**Data analysis**

Validity and reliability are the key concepts for measurement quality. Our conceptual framework uses definitions of validity and reliability as described in the *Standards*.[49] The American Educational Research Association (AERA), the American Psychological Association (APA), and the National Council on Measurement in Education (NCME) have jointly developed the *Standards*. These Standards were, therefore, in existence when the instruments in the sample were published. The *Standards* provide criteria for evaluating tests, testing practices, and the effects of test use, where "test" is broadly construed to include affective scales, surveys, and traditional knowledge tests.[49]

### ***Sources of Validity Evidence***

Validity refers to "the degree to which evidence and theory support the interpretations of test scores entailed by proposed uses of tests".[49,51–53] While the concept of validity may seem straightforward, multiple sources of validity evidence are relevant. These sources of evidence illuminate different aspects of validity, yet they all represent the unitary concept of validity.[49,53–55] Checking validity evidence each time an instrument is used is important, because, as Nunnally[21] indicates, problems with measurement quality arise not only from the instrument itself but also from sampling error associated with people. In other words, the same instrument can produce different validity results for different groups of people. In this study, three sources of validity evidence as described in the *Standards* were gathered: evidence based on test content, response processes, and internal structure.

Validity evidence is only one aspect of an instrument's quality. To obtain meaningful test scores, there should be some degree of stability in test-takers' responses if the measure is given multiple times.[49] If the same test yields markedly different scores for each administration to the same individuals, we cannot reliably interpret those scores. An instrument must measure the construct of interest with some degree of consistency if we hope to make valid interpretations. Therefore, examining reliability evidence is important.

### ***Sources of Reliability Evidence***

Reliability concerns the consistency of a measure and procedures used to score that measure when it is administered to the same individuals multiple times.[49,59] Having consistent scores over multiple occasions ensures that the scores can be reliably obtained and are not due to chance. For many reasons, including changes in effort and test anxiety, obtaining perfect reliability of scores over multiple occasions is unlikely.[49] However, because users cannot confidently make generalizations from unreliable data, reliability information should still be reported.

According to the *Standards*,[49] reliability information may be reported as variances or standard deviations of measurement error, coefficients, or test information functions based on item response theory. The instruments in the sample report reliability information based on coefficients. The evidence is based on replicate administrations and internal consistency of the instrument, each of which is described in this study.

## Research methods employed -Quantitative full study

### Participants

Chemists from academia, industry, government, and other chemical sectors were invited to participate in this online survey. Only chemists that hold a doctorate degree in chemistry and related field were investigated in the project. All individuals on a master list were invited via email. The master list of the universities or colleges, companies, governments, and individuals were compiled in two ways. First, for research faculty and teaching faculty at universities or colleges, the contact information is available online, the emails were compiled easily by scraping departmental websites. The email addresses of 5450 faculty members from 207 institutions were collected in a master list. The institutions include 2-year college, community college, 4-year liberal arts college, 4-year comprehensive college, and 4-year research college.

Second, contact information of industrial chemists and chemists in government positions is less likely to get from the website. Representatives from a list of companies and participants of the qualitative phase were contacted with a letter of our research aim and the request of distributing the invitation to their colleagues and collaborators by snowball sampling. The purposeful sample was designed to invite chemists from a variety of position types.

In order to ensure enough participants were recruited in each "group" to achieve statistical power. The power analysis was conducted by G*power software with the condition of F-test for ANOVA, $\alpha = 0.05$; power = 0.8. Small, medium, and large effects for ANOVA are 0.1, 0.25, 0.4, respectively. The results of qualitative study indicated that chemists in different job sectors require different sets of knowledge and skills, we expect to find large effect as opposed to small or medium effect. Thus, the target sample size 21 in **Table 5** reflects the minimum number of participants per group needed to detect large-sized effects for three types of job sectors (academia; industry; other).

The minimum target sample number is 63 (21*3 = 63), but as many respondents to the survey as possible were attempted to maximize the generalizability.

**Table 5. Power Analysis Results**

| Test | Small Effect* | Medium Effect* | Large Effect* |
|---|---|---|---|
| ANOVA (3 groups) | 322 | 53 | 21 |

*Small, medium and large effects for ANOVA are 0.1, 0.25, and 0.4, respectively

Additionally, the participants should represent the national distribution of broad sectors, the target number of participants from each sector were determined by the national distribution of chemists in different sectors and power analysis (**Table 6**), the minimum target sample size is 210. But it is difficult to get responses from industry, academic faculty are over-represented in our real sample.

**Table 6. Target Sample and Real Sample Distribution**

| Sector | National distribution | Quantitative sample | Our sample |
|---|---|---|---|
| Academia | 37-50% | 105 (50%) | 308 (75%) |
| Industry | 43-56% | 84 (40%) | 72 (17%) |
| Other | 8-10% | 21 (10%) | 32 (8%) |
| Total | | 210 (100%) | 412 |

**Data collection**

In order to reach these chemists, the survey was distributed via email to chemists in academia, industry, government as well as other job sectors. The survey was also posted on chemistry relevant social media such as twitter, LinkedIn. $10 Amazon gift card was given if participants take the survey and follow-up interview; $20 Amazon gift card was given if participants take survey twice as well as follow-up interview. In addition, there was 1:500 chance to win $100 for all participants. A total of 412 responses were received from academia, industry, government and other job sectors (**Table 7**). Among them, there were 152 female, 256 male, and 4 unknowns. Participants of different races were included, the majority of participants were white. Compared to the national distribution, our sample roughly represents the population of doctoral chemists.

**Table 7. Sample Distribution in Full Survey**

| | | ***N* = 412** |
|---|---|---|
| Sex | Female | 152 (36.9%) |
| | Male | 256 (62.1%) |
| | Unknown | 4 (1.0%) |
| Job sector | Academia | 308 (74.8%) |
| | Industry | 72 (17.5%) |
| | Other | 32 (7.8%) |
| Race | Asian | 67 (16.3%) |
| | Black/African American | 10 (2.4%) |
| | Hispanic/Latino | 8 (1.9%) |
| | Native Hawaiian/Pacific Islander | 1 (0.2%) |
| | White | 311 (75.5%) |
| | Other | 13 (3.2%) |

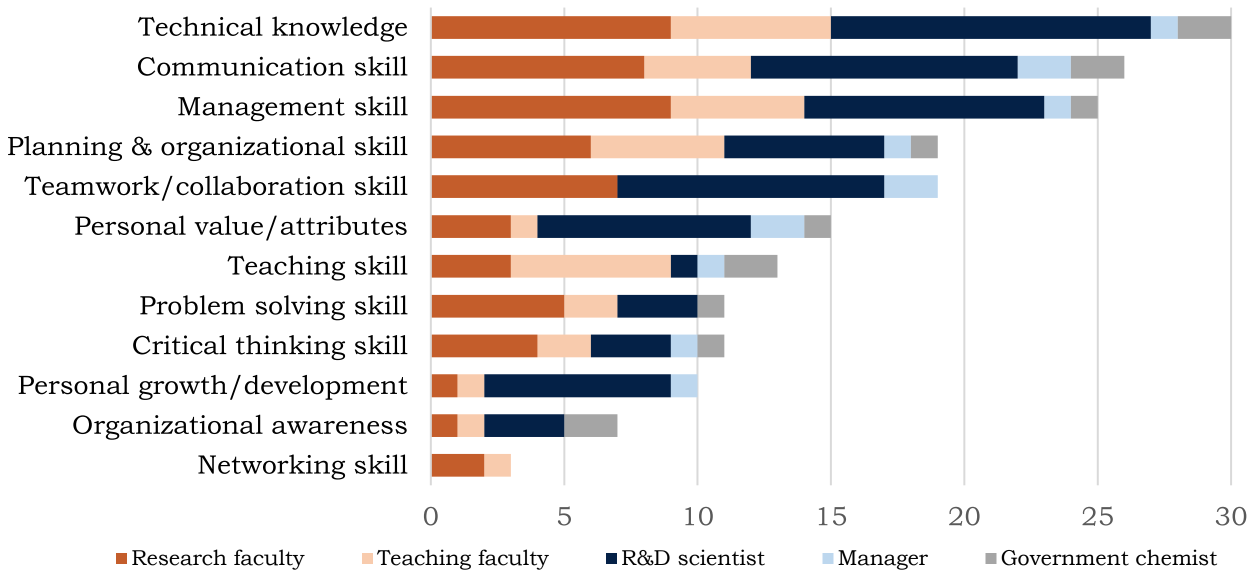
# CHAPTER 3: RESULTS AND DISCUSSIONS

## Results and discussions -Qualitative study

After thematic coding, 12 major themes emerged relating to the knowledge and skills chemists believed to be required for their careers (**Figure 4**; see Appendix 3 for definitions of these knowledge and skills). In this figure, orange, blue, and green bars indicate different chemical sectors - academia, industry and government - and the darkness of color indicates the different work functions within each job sector. Chemists were included if they mentioned this knowledge or skill at least one time throughout the first two phases of the interview (i.e. the participant had to independently bring up the knowledge or skill). From the distribution of job sectors in each of the twelve knowledge and skills, it is clear that technical, communication, management, planning/organizing, personal value, teaching, and critical thinking are ubiquitously required for chemists in all three chemical sectors, but it also seems apparent that each type of chemist can require different set of skills and knowledge.

In the following subsections, each theme is broken down and trends are discussed further. With a large number of codes in a specified hierarchical structure, referencing all codes is not viable. Partial codes are shown in **Table 8**, and the entire codebook can be found in Appendix 3. The following nomenclature is used to help align our claims: ([code name], # / # / #). In this system, the brackets contain the code name, and the three values separated by slashes correspond to the number of academic faculty, industrial chemists, and government chemists, respectively, that described the particular code. As an example, ([data analysis], 7 / 3 / 2) means that 7 / 15 academic faculty, 3 / 14 industrial chemists, and 2 / 2 government chemists mentioned the importance of data analysis skills in performing their jobs.

**Figure 4. List of Knowledge and Skills that were Mentioned in the Interviews**




**Technical knowledge & skills**

Unsurprisingly, all but one chemist mentioned that technical chemistry knowledge and skills were essential for their jobs. This foregone conclusion simply confirms that chemists need to know basic and/or advanced chemistry, experimental procedures, and instrumental know-how to perform their jobs as chemists. While some chemists elaborated which types of technical knowledge and skills would be more useful than others, our primary intent was to focus on non-technical skills for this study.

**Communication skills**

Communication skills consist of the ability to both give and receive different forms of information for the purposes of oral and written communication. A total of 26 participants described written and/or oral communication skills as a particularly important competency in the workplace. Across the board, most chemists thought of communication skills as important, but differences emerged as these chemists described subskills of communication. Industrial chemists emphasized the importance of general talking skills more than chemists in other sectors ([general talking skills], 3

/ 8 / 1) and were the only ones to discuss the importance of knowing the background of their audience during a conversation ([knowing the audience], 0 / 5 / 0) while emphasizing interpersonal understanding ([interpersonal understanding], 2 / 7 / 0). In contrast, written skills were brought up most frequently by academic faculty ([written skills], 11 / 2 / 2), with a notable skew towards research faculty compared to teaching faculty (8 research faculty and 3 teaching faculty). Faculty mostly related quality writing to presenting an organized piece of work ([being organized], 6 / 1 / 0). Beyond being organized, no consensus was reached in the sample for other characteristics of quality writing. However, it is likely that the products of what is written in each work function drove the knowledge and skills needed. Research faculty communicate complex experimental details when writing grant proposals or scientific papers, leading them to discuss writing explicitly ([writing explicitly], 4 / 2 / 0), concisely ([writing concisely], 3 / 2 / 0), accurately ([writing accurately], 3 / 1 / 0), and meeting the specific formatting and norms ([meeting the requirements], 3 / 1 / 1). Teaching faculty mentioned the need for knowledge and skills to write recommendation letters for students and laboratory materials for TAs. Industrial & government chemists stated that they wrote summary reports and other products to non-technical audiences. These chemists did not exhibit clear information as to what specific knowledge and skills they required, except knowing the background of their audiences ([knowing the audience], 0 / 1 / 1).

**Management skills**

Management skills are the abilities that a manager, supervisor, advisor, or instructor should possess in order to complete specific tasks in an organization. Chemists in different positions all reported management skills as necessary. However, each type of chemist tended to define the management skill differently (detailed codes and descriptions of each code can be found in Table 8), so that thematic analysis was not efficiently conducted unless the specific context of the chemists' job sector and work function was properly accounted for (thus aligning with our theoretical lenses).

**Table 8. Partial Codes and Descriptions of Management Skills and Subskills**

| Management Skill | Subskills | Description |
|---|---|---|
| Lab management for research faculty | Supervising skill | This refers to giving students guidance and direction, and making sure that they can meet the degree requirement |
| | Training students | This refers to teaching students new techniques, writing skills, or other knowledge and skills. Sometimes they may not teach directly, but students can learn from them. |
| | Securing funding | This includes securing external funding and keeping track of the budget |
| | Overseeing project | This refers to monitoring the project progress to make sure it runs smoothly in the proper timeline |
| | Organizing lab | This refers to making sure all equipment in lab is working, and organizing team |
| Management skill for teaching faculty | Managing TA | This includes setting goals, training TAs to make sure they are well-prepared |
| | Managing students | This refers to manage students in their classes or in labs |

| | | |
|---|---|---|
| | Supervising lab manager | This includes training lab manager and setting standard procedures for them. |
| Project management | Managing people | This refers to understanding what people need, require and accept, and managing them efficiently. |
| | Managing time | This refers to figuring out what needs to be done in what order and how quickly it can be. |
| | Setting goals | This includes knowing the objective and the mission of a project. |
| | Managing budget | This includes knowing the cost, resources, sponsors, and keeping an eye on how money has been spent. |
| | Patent management | This refers to management of patents and intellectual property. |
| | Risk and uncertainty management | This refers to reducing risk and uncertainty of a project. |

***Academia: Research faculty' view of management***

All nine research faculty reported that management skills were essential for their jobs. The lab management in academia only included the responses of faculty doing research as primary duty. Research faculty defined management skills as supervising students ([supervising skills], 9 / 0 / 0), securing funding ([securing funding], 4 / 0 / 0), overseeing projects ([overseeing projects], 4 /

0 / 0), and organizing labs ([organizing labs], 2 / 0 / 0). Jack (pseudonym), a research faculty, saw his supervisory role as guiding and motivating students ([motivating students], 3 / 0 / 0).

*"I think knowing how to motivate, and how to direct, how to apply the right level of supervision, it requires practice, it requires patience." ~ Jack*

Several faculty used a more cognitive approach to training ([training students], 7 / 0 / 0) that involved working with students to teach them key technical skills:

*"I think you have to work with the student, you have to be able to sit down with them and go over in detail the data you're collecting, and what it all means, and they have to be able to understand what you're saying, and learn from my expertise. [Faculty] have to share that and get the students to think critically, and think about what the results actually mean, and not to just accept that they have something really interesting when they don't." ~ James*

***Academia: Teaching faculty' view of management***

The management skill for teaching faculty contained the responses of five teaching faculty, but research faculty who had teaching as secondary positions were not included in this category. Generally, management skills for teaching faculty included managing TAs for labs, students in their classes, and lab managers who were working with them. However, there were not many overlapping ideas when discussing how to manage these various parties. When managing TAs, some instructors found it necessary to set goals for them ([setting goals], 2 / 0 / 0) so that TAs would know what they should do for the lab. Others needed skills to give orientations for TAs and gave them feedback to make sure TAs were well-prepared ([training TAs], 3 / 0 / 0). One particular faculty expressed several of these ideas, which generally relied on other abilities such as teaching and presentation skills:

*"These are the objectives of what is going to happen this week, and here's what you need to know. we give them the class, and then they have a whole day to prepare, and then they have to demonstrate to us how they would teach the lab that has been assigned to them. So they are observed, and they get feedback to make sure that they're delivering those materials in the way that we expect them to do it." ~ Emily*

In a smattering of other knowledge and skills, one instructional faculty claimed that an organized class was important for management ([managing students in class], 1 / 0 / 0). Having a class syllabus, class policies, and realistic expectations for the students were also brought up by the teaching faculty. In general, instructional faculty had a variety of other responsibilities or services such as advising students and supervising lab managers. These responsibilities required additional knowledge and skills, the subskills for which were included in the codebook (Appendix 3).

***Industry & Government: Industrial & government chemists' view of management***

Many industrial (and the two government) chemists believed that some form of management skills were required for their careers and described them in varying ways (Table 4). The management skill in industry was typically project management, which related to the design and carrying out of a specific project. Many industrial chemists primarily focused on managing people in a broad sense ([managing people], 0 / 8 / 0), managing time ([managing time], 0 / 7 / 0), and setting goals ([setting goals], 0 / 5 / 0). Chemists focused less frequently on managing budgets ([managing budget], 0 / 2 / 1), keeping patents ([patent management], 0 / 2 / 0), and checking risks and uncertainty ([risk & uncertainty management], 0 / 2 / 0). Budget management was the only thing that was mentioned by government chemists when the participant talked about management skills. Managing people generally depended on interpersonal skills ([interpersonal understanding], 0 / 7 / 0), and interestingly, the two participants that were managers mentioned only this subskill when describing management. Judy (pseudonym), spoke about the realities of understanding the world from different perspectives. This quote reflected some qualities of interpersonal skills including a general respect for others ([respecting people], 0 / 2 / 0), empathy ([having empathy], 0 / 1 / 0), and ability to motivate people ([motivating people], 0 / 1 / 0).

*"Sometimes your projects may be important to you, but they may not have as much prioritization with other people…So finding that balance between patience and kind of influencing or pushing people along can be kind of frustrating sometimes, but it's something that's a reality." ~ Judy*

Industrial chemists emphasized the importance of managing time. The chemists spoke about the knowledge and skills required for establishing timelines ([establishing timelines for the project], 0 / 6 / 0), general balancing time between projects ([balancing time], 0 / 3 / 0), and knowing when to abandon a project ([knowing when to quit], 0 / 1 / 0). The broad skills of managing time were reflected in the following quote.

*"...you have to figure out what needs to be done in what order it needs to be done in, and how quickly it needs to be done to enable the project to succeed... you have to know all the pieces that go into this, what takes time, what doesn't, what's going to be the rate-limiting step, and what won't be, what's critically important, and what isn't important, things like that." ~ John*

**Other knowledge and skills**

Other knowledge and skills that chemists used in their positions were also identified. **Table 9** showed the significant knowledge and skills that were commonly mentioned by chemists within each work function.

Research faculty reported the need for teamwork skills when working with other collaborators such as planning ahead of time, balancing time between different duties, and trouble-shooting/being creative when they solve a problem. Problem-solving skills were only emphasized by research faculty. Teaching faculty expressed the need for good teaching skills, involving course preparation and teaching strategy implementation. In addition, they required planning & organizational skills to manage time and organize materials. Both R&D scientists and managers in industry described teamwork skills because they worked with people within or outside of the group, department or company. Personal value was reported by most industrial chemists, but this was not the case with chemists in other job sectors. Furthermore, R&D scientists mentioned personal growth more frequently than other types of chemists, which involved having willingness to learn new things and keep practicing after training. Both government scientists talked about teaching skills when training new hires, which included different contents for teaching faculty in academia. They followed standard procedures to provide new employees hands-on, work-based training. In order to complete daily tasks successfully, they also require planning & organizational skills to be efficient, interpersonal skills to work with colleagues and the general public, as well as problem-solving skills to solve technical and non-technical problems.

**Table 9. Other Significant Skills and Values by Sector**

| Skills and Values | Academia | | Industry | | Government |
|---|---|---|---|---|---|
| | Research faculty | Teaching faculty | R&D scientist | Manager | R&D scientist |
| Teamwork skills | + | − | + | + | − |
| Planning and organizational skills | + | + | − | − | + |
| Personal value | − | − | + | + | + |
| Teaching skills | − | + | − | − | + |
| Problem-solving skills | + | − | − | − | + |
| Personal growth | − | − | + | − | − |

**Results and discussions-Survey development**

**Survey development**

The survey given to participants included two parts. One part was the background check of participants. Participants' gender, race, Ph.D. area, work year and job sector were assessed in this part (**Table 10**), in order to see if there is any knowledge or skill differing among groups. The analysis is limited to chemists with a doctorate in the U.S. so that the data could be compared to the U.S. surveys on the demographics.

**Table 10. Background Information Options in Pilot Survey**

| | | | | | | |
|---|---|---|---|---|---|---|
| **Gender** | | | | | | |
| Male | Female | Prefer not to answer | I prefer to self-identify | | | |
| **Race / Ethnic origin** | | | | | | |
| Hispanic/Latino | White | Black / African American | Native Hawaiian / Pacific Islander | Asian | American India / Alaska Native | Other |
| **Ph.D. area** | | | | | | |

| Analytical Chemistry | Biochem | Organic Chemistry | Inorganic Chemistry | Physical Chemistry | Chemistry Education Research | Other |
|---|---|---|---|---|---|---|
| **Work year** | | | | | | |
| **Job sector** | | | | | | |
| Academia | | | | | | |
| 2-year College | Community College | 4-year Liberal Arts College | 4-year Comprehensive College | 4-year Research College | | |
| Industry | | | | | | |
| Pharmaceutical and Medicine Manufacturing | Chemical Manufacturing | Petroleum and Coal Products Manufacturing | Health and Personal Care Manufacturing | Oil and Gas Extraction | Other Specialty Trade Contractors | Other |
| Government | | | | | | |
| Federal Government | National Lab | State or Local Government | Other | | | |
| Other | | | | | | |

The other part included items that were derived from the results of the previously discussed qualitative study and literatures. The participants were asked to rate the agreement of a list of knowledge and skills using a six-point Likert-type scale and a separate option of *Not Applicable*. The Likert-type scale is: *(1) Strongly Disagree, (2) Disagree, (3) Slightly Disagree, (4) Slightly Agree, (5) Agree and (6) Strongly Agree.* The scale is symmetric and balanced for giving both positive and negative end, as well as giving participants flexibility to choose from the options. Six-point Likert scale is used to increase response rate and response quality along with reducing respondents' frustration level. A higher point Likert scale makes it more time consuming for participants to make decisions. Having six points tends to be a good balance between having enough points of discrimination without having to maintain too many response options. In most cases, a neutral option, such as *Neither Agree nor Disagree*, is given. But this option will not be included in this survey because we will assign each scale to a value, *Neither Agree nor Disagree* will be the same value of the average of (Strongly/Somewhat) *Agree* and (Strongly/Somewhat) *Disagree* when data analysis is performed, but it cannot be treated as the average of positive opinion and negative opinion. In order to avoid misinterpretation of the results, *Not Applicable* option is provided for participants, and was analyzed separately.

Items of this survey met the research objectives and corresponded to the themes that were emerged from the qualitative study. Taking the assessment of management skills as an example, the evidence of chemists in different job sectors having different understandings of management skills had been revealed in the qualitative study. Thus, a single item of rating the agreement on the importance of management skills was not appropriate. It is a broad concept, it was broken down into several sub questions. A total of 14 specific questions below had been designed to evaluate different aspects of management skills.

1. motivate/inspire others
2. utilize the influence I have over others to see projects through
3. keep records of the progress of different projects
4. plan out and track the progress of multiple projects
5. identify potential sources of funding
6. identify the challenges and constraints of obtaining financial resources
7. persuade others within my organization to allocate financial resources
8. persuade others outside of my organization to allocate financial resources
9. conduct "book-keeping" of a budget (i.e. track revenue, expenses)
10. foster group facilitation
11. assess someone's work and provide feedback
12. train other employees, interns, or assistants to conduct a certain job
13. set goals within a group for a project or issue
14. minimize safety risks

For example, items 5-9 evaluate financial management, which was an important part of management skills. They were derived from the quotes of interviews and the code book that were developed in qualitative study. The quote below was from the interview of an industrial chemist, showing that keeping track of money, estimating how much money will be spent, and identifying the potential sponsors were important for financial management. Thus, items to evaluate where (item 5) and how (item 6-8) chemists obtain financial support, as well as how (item 9) chemists keep budget can be developed.

*So budget management is part of discipline, being organized,* ***keeping track of the money that's being spent****,* ***being able to estimate how much money*** *or* ***how many resources you need*** *at* *the beginning. And then* ***keep an eye on that money****, so that you are not overspending, and if you are going to need additional resources, you know* ***how to bring that to the attention of the project sponsors****. ~James*

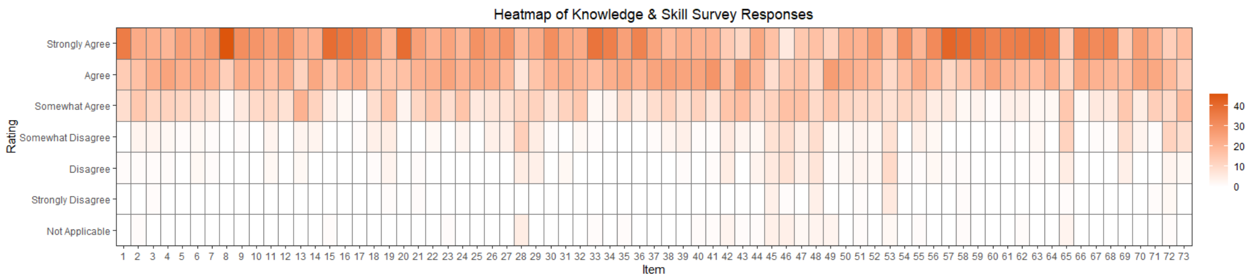
The evidence collected in the qualitative study indicated that each type of chemist required different sets of skills and knowledge, and even for the same broad knowledge or skill, participants defined them differently. In order to help design the survey further, how chemists in different job sectors responded to each of the items based on the results of the qualitative research were taken into consideration. For example, responses would differ among groups for item 5. Most of research faculty might agree with it, because participants in qualitative study mentioned their responsibilities of securing funding to run their research groups. Most of teaching faculty might not have to apply for funding, they probably might disagree with this item. Chemists from industry or government might agree or disagree with this item depending on their job duties.

**Pilot study**

The pilot study addressed the two research questions: (1) what items should be modified or removed from the doctoral chemist's knowledge and skills inventory and (2) what validity and reliability evidence exists for the knowledge and skills inventory.

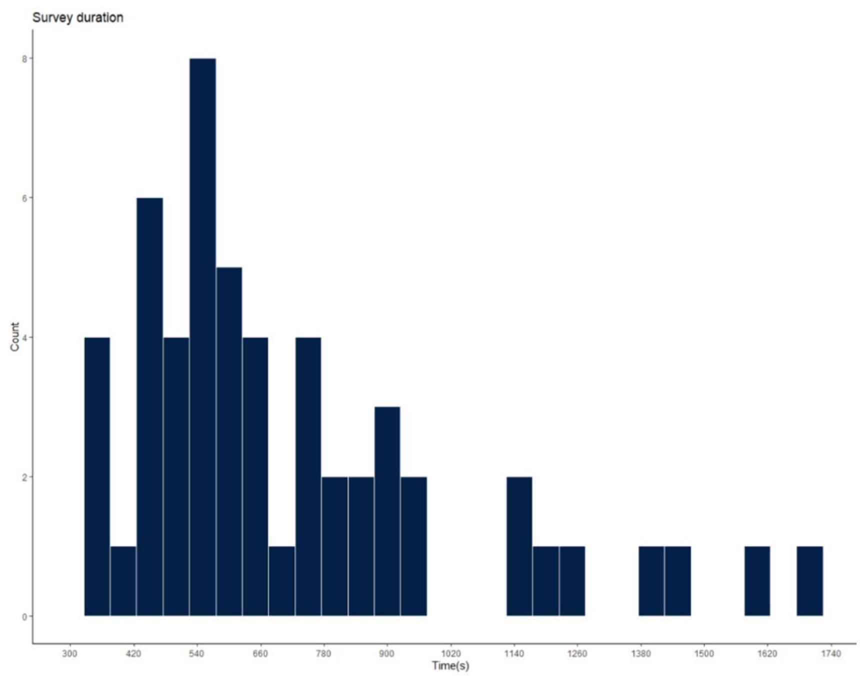
The heatmap shows the overall knowledge and skills response distribution (**Figure 5**). The darker shade of orange represented the more counts of a specific rating. In this figure, the darker shade located at "*Strongly Agree*" or "*Agree*" for the majority of the survey items. It indicated a dominance of high ratings, meaning that the participants required/valued most of the knowledge and skills in the survey list. Only a few items contain responses on "*Not applicable*".

**Figure 5. Heatmap of Knowledge and Skill Survey Response in Pilot Study**




Additionally, time was recorded to evaluate how long it took to complete the survey (**Figure 6**). From the histogram, most of the participants can finish the survey in 15 minutes.

**Figure 6. Histogram of Recorded Time to Complete the Survey**




***Validity evidence***

Evidence based on test content

According to the *Standards*[49], "test content refers to the themes, wording, and format of the items, tasks, or questions on a test, as well as the guidelines for procedures regarding administration and scoring",[49] which is consistent with the definition of content validity used in other studies.[57,58]

Evidence based on test content addresses the relevance and representativeness of test content in light of the intended construct.[59] Establishing evidence of content validity is crucial, as interpretations of test scores concerning a particular domain are only valid if the test adequately captures that domain.

To generate evidence based on test content for this survey, chemistry education experts determined whether the items appropriately sample the domain of interest,[48] with a focus on sufficient and accurate representation. In this study, four chemical education researchers judged the level of representativity and exhaustiveness of the survey items. Taking financial management as an example. At first, a question was constructed -- convince people to give me money. The words "people" and "money" were too vague in this item, then it was changed to "persuade others in an organization to allocate financial resources" giving some specific descriptions of money and whom to convince. However, it was still unclear that what kind of organizations they should persuade. After several rounds of discussions between chemistry education researcher, this survey item was split into two questions – "persuade others within the organization to allocate financial resources" and "persuade others outside of the organization to allocate financial resources".

The observed test scores are inseparably linked to how participants interpret and respond to the items. In order to have further evidence of validity, the test must also demonstrate the ability to sample the cognitive processes required to answer items related to that domain.[25] Therefore, it is important to examine evidence based on response processes.

Evidence based on response processes

According to the *Standards* [49], evidence based on response process refers to "evidence concerning the fit between the construct and the detailed nature of performance or response actually engaged in by examinees" (p.12). The *Standards* provide few indications for obtaining evidence about the response processes:

*Questioning test takers about their performance strategies or response to particular items…Maintaining records that monitor the development of a response to a writing task… Documentation of other aspects of performance, like eye movement or response times* (p. 12).

It indicates that obtaining evidence based on response processes combine who provides the data (participants) with the data itself (responses). Response processes are the underlying cognitive activities that participants practice to answer a question.[61] Examining this type of evidence ensures that the processes being used by test takers to answer survey questions are those intended by the test developer. This type of evidence can be obtained by analyzing response processes.[49]

Cognitive interviews are useful for examining response processes. These are in-depth interviews used to get feedback from participants about items on an instrument,[62] and provide insight into participants' thought processes when responding to survey items. Validation interviews allow the survey developer to explore in detail the participants' thinking and understanding of the items when they respond in certain ways to the individual item.

In this study, a total of 19 doctoral chemists from academia, industry or government participated in a brief validation interview to assess readability. For items selected, we assessed participants' understanding of what the item is asking; their interpretations of key words and phrases; alignment of current thoughts to response options; and satisfaction with how the item matches their beliefs/thoughts (See Appendix 7 for example transcript). Items with wording issues were either rewritten or deleted from the survey list. After analyzing the validation interviews, there were eight participants that mentioned it was unclear whether the item clearly portrays my profession. To avoid the misunderstanding of this item, the item 55—understand my profession fully was deleted from the survey list. In addition, there were two participants that had an issue of understanding the item 43-foster group facilitation. By analyzing the reasons of responding to this item, it was modified to "foster good work climate and assist group members to accomplish tasks".

Evidence based on internal structure

According to the *Standards*[49], evidence based on internal structure refers to "the degree to which the relationships among test items and test components conform to the construct on which the proposed test score interpretations are based" (p. 13).

Evidence based on internal structure addresses how well the instrument generates robust measures of the desired construct. In order to generate the robust measures of a latent construct, a specific structure of the underlying instrument derived data must be present. This structure may be considered as a benchmark for productive measurement. And only if this structure is present, can the latent measures generated be interpreted.

The internal structure of an instrument concerns the relationships among instrument items.[49] A conceptual framework for an instrument may prescribe the intended construct as unidimensional or multidimensional; regardless, the item relationships should be consistent with the underlying structure. Evidence based on internal structure establishes the degree to which the items on the instrument conform to the hypothetical construct.[63] In this study, factor analysis was adopted to search for the structure among the set of knowledge and skills.

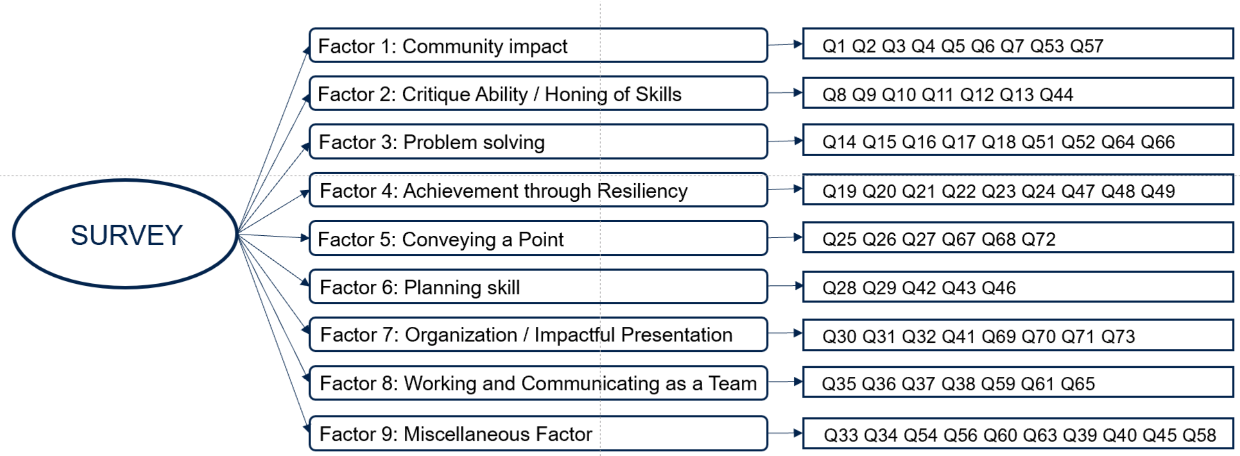
Factor analysis is a technique that transforms the correlations among a set of observed variables into smaller number of underlying factors, it is useful for identifying groups of items which survey questions that are strongly correlated, these groups of strongly correlated items represent some reflective factor because they move together consistently.[64] The assumption is that items measuring the same construct will load on the same "factor" and item scores will be correlated with one another.

Exploratory factor analysis (EFA) is used to explore the underlying factor structure of a set of measured variables without imposing a preconceived structure on the outcome. EFA is driven only by data, not theory. The number of factors is not specified a priori. Researchers do not have a hypothesis; they need to explore the relationships among variables to identify patterns. Therefore, the number of factors to be estimated is not specified from the beginning, it is determined based on what the data showing.

In this study, there were 60 responses obtained. Each survey item (knowledge or skill) served as one variable; factor analysis transformed the correlations among a set of observed variables (survey items) into smaller number of underlying factors. The results can guide us to rewrite or remove the problematic items from the pilot survey.

For this survey, after conducting EFA with changing different factor numbers, factor extraction algorithms and factor rotation methods, a structure of nine factors was interpreted (**Figure 7**). See Appendix 8 for factor analysis output and Appendix 9 for factor structure. A factor is a group of items that measure one similar construct. The first eight factors can be labeled as community impact, critique ability/ honing of skills, problem solving, achievement though resiliency, conveying a point, planning skill, organization/impactful presentation, and working and communicating as a team. All the other items were combined to the miscellaneous factor, it indicated that these items were possibly on the drop list or needed to be rewritten.

**Figure 7. Factor Structure of Knowledge and Skill Survey Responses**




***Reliability Evidence***

Evidence Based on Internal Consistency

Internal consistency is a measure based on the correlations between different items on the same subscale on a survey. It measures whether several items that propose to measure the same general construct can produce similar scores. Essentially, participants who respond to one survey item in a particular way will be more inclined to respond to other similar items in the same way. That is, items that are related or measuring the same construct will be correlated,[40] providing a measure of internal consistency.

Coefficient α[68] is the most commonly used measure of internal consistency reliability,[69] that is, how closely related a set of items are as a group. Although it has been critiqued for underestimating test reliability[47] and for having little value when used by itself,[70] the usefulness of coefficient α to estimate an instrument's internal consistency has been well documented.[69] Typically, the cited desired value is 0.7 or above;[63] however, there is no particular value of α that is considered to be acceptable. For this survey, an instrument with subscales has the 0.56-0.82 α value for each subscale.

In addition, item total correlation was calculated to support the internal consistency reliability of the instrument. The item total correlation is a correlation between the item score (e.g., 6 or 5 for Likert-type scale) and the overall assessment score. It is expected that if a participant gets an item high rating, in general, should have higher overall assessment scores than participants who get this item low rating. For our data, the item total correlation is 0.47-0.74, showing satisfied internal consistency. In this study, both coefficient α values and item total correlation showed fair to good internal consistency within each subscale.

Evidence Based on Temporal Stability

To ensure that a test consistently measures test-takers' performance on the construct of interest, test administrations in different occasions are needed. Gathering this evidence involves administering the test to the same group of individuals twice and calculating the correlation between the scores from the first and second administration.[49,65,66] This method of estimating reliability assumes that there will be some degree of stability in the scores obtained over repeated test administrations. This assumption is warranted only when there has been no treatment or maturation between administrations that would be expected to change the respondents' status with respect to the construct of interest.

There are several different measures available for estimating test-retest reliability. The Pearson's correlation coefficient has been the most common technique for assessing reliability between the two sets of test scores. If a high (>0.8) and statistically significant correlation coefficient is obtained, it indicated that not many responses have changed from Time 1 to Time 2 with regard to what is being measured, and therefore, the instrument is deemed to be sufficiently reliable.

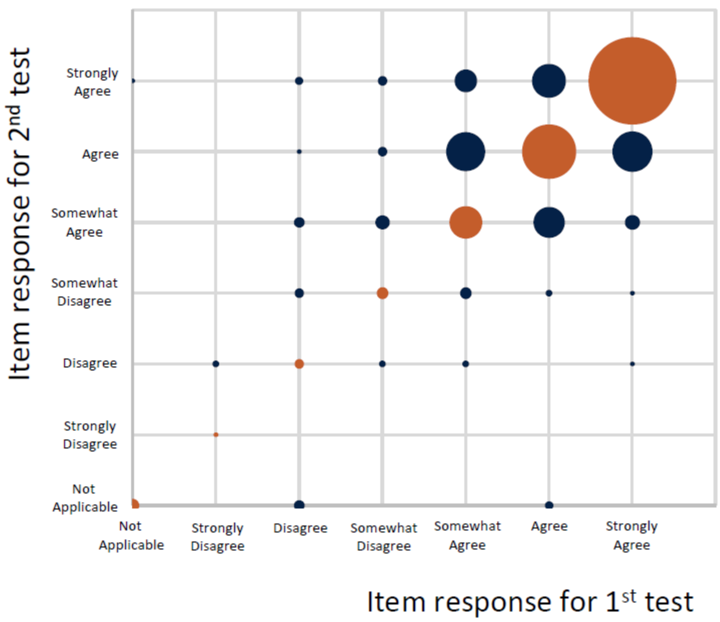
In order to evaluate the temporal stability, participants were asked to take the survey again to determine test-retest reliability. To calculate the sample sizes needed to detect a relevant simple correlation with specified significance level and power, following hypotheses were used: $H_0$: $\rho = 0$, $H_a$: $\rho = r \neq 0$, where significance level $\alpha = 0.05$; power of the test $1-\beta = 0.8$; sample correlation $r = 0.8$. The sample size needed for test-retest reliability can be estimated, N = 10.

In this study, there were 12 retest results obtained. The data was used to calculate the test-retest reliability on the total score level and item score level. On total score level, all responses for all survey items from a participant were summed up as one score, there were two total scores for the first and the second tests, respectively. To calculate the test-retest reliability, the Pearson's correlation coefficient was assessed between the two test scores for 12 participants, N = 12. The Pearson's correlation coefficient on total score level is 0.94, which is very high and indicates the consistency of scores over replicate administrations.

On item score level, each survey item response of the first test was compared to the same survey item response of the second test for a participant. Thus, there were two sets of item scores for the first and the second tests, respectively. To calculate the test-retest reliability on item score level, the Pearson's correlation coefficient was computed between all the item scores of the first test and the second test, thus there were 876 points in total (N = 12*73 = 876). The Pearson's correlation coefficient on item score level is 0.69, which indicates satisfied temporal stability of the instrument.

To visualize the consistency of the item scores for two administrations, a bubble plot was created (**Figure 8**). In the bubble plot, the orange bubble represents the same item responses for the first test and the second test, while the blue bubble represents the different item responses for the first test and the second test. There were 876 points in total and there were 549 exact same item responses for test-retest comparison, the percentage of same rating was 62.9%. The results above indicated good temporal stability of this survey.

**Figure 8. Test-Retest Reliability on Item Score Level**



## Results and discussions-Quantitative full study

### Data processing

The Qualtrics system automatically records each respondent's survey completion duration with a starting date/time and an ending date/time—we removed participants who completed the survey in less than five minutes. We also checked respondents who marked all questions with the same option on the Likert-type scale or have large proportion of missing values (e.g., > 90%). A total of six participants with large percentages of missing values were deleted, as these individuals may not have taken the survey seriously and imputing that much missing data can be problematic.

A person's attention may change during the survey, careless response or error may occur. There were two focus check questions designed in the survey. When analyzing the data, only observations with correct responses for both focus check questions were kept for the further data analysis. There were 29 data dropped because of the participants' careless response. Thus, a total of 383 observations was obtained.

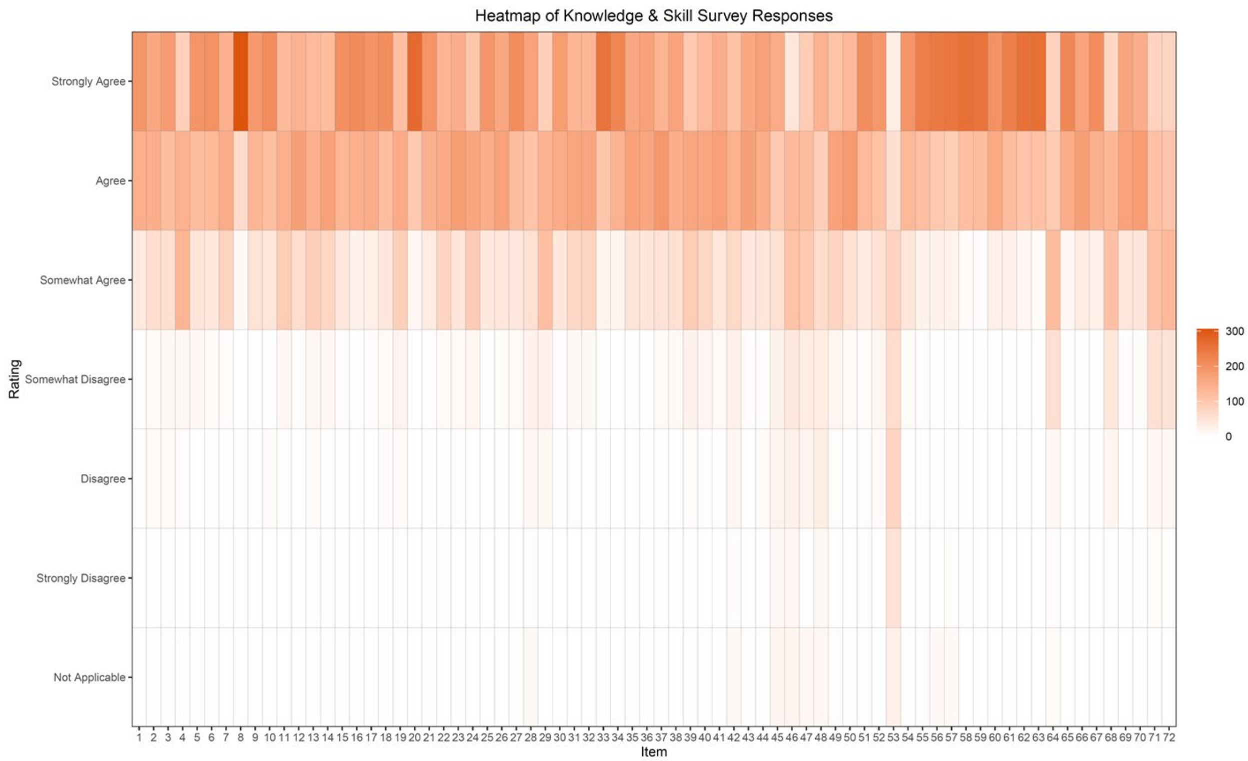
The survey data contained a proportion of missing values, which would be removed from the analysis or imputed by different approaches. A direct approach to handle missing data is to exclude them, but the results can yield bias or potential issues because the sample of observations that have no missing data might not be representative of the full sample. Rather than removing variables or observations with missing data, missing value imputation can be conducted. A variety of imputation approaches (such as hot-deck imputation; approximate Bayesian bootstrap imputation) can be used to predict the nonresponse data. In this dataset, there were 47 missing values, the proportion of them is 0.17%. The proportion of missing values across the data set is relatively low (< 5%) and the data are deemed to be missing at random (i.e. there is no systematic reason for the missing responses), the methods used for estimation of the missing values will have only a minor impact on the results. The observations with no missing data were evaluated as references and were used to impute the missing values. Each item for each participant was treated as one imputation cell, and missing data was imputed by calculating the median of the item score.

**Data analysis**

Technically a Likert scale is ordinal, but researchers often assign values to each option and treat data as interval variable, which is a type of continuous variable. In our case, 1 was assigned to "*Strongly Disagree*", 2 was assigned to "*Disagree*", 3 was assigned to ''*Somewhat Disagree*'', 4 was assigned to ''*Somewhat Agree*'', 5 was assigned to "*Agree*", 6 was assigned to ''*Strongly Agree*'', and 0 was assigned to "*Not Applicable*".

The heatmap (**Figure 9**) can show the overall knowledge and skills response distribution. The darker shade of orange represented the more counts of a specific rating. In this figure, the darker shade located at "*Strongly Agree*" or "*Agree*" for the majority of the survey items. It indicated a dominance of high ratings, meaning that the participants required/valued most of the knowledge and skills in the survey list. Only a few items contain responses on "*Not applicable*".

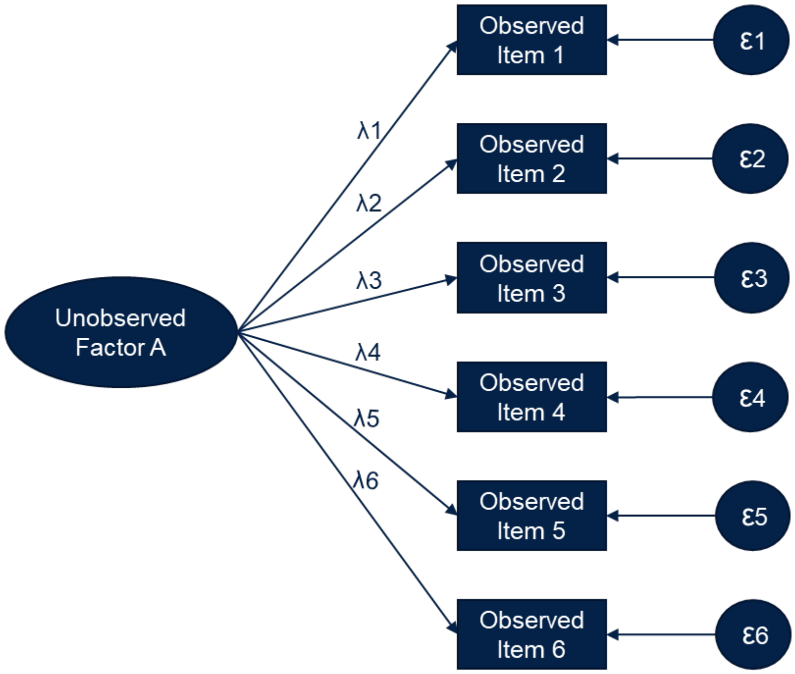
**Figure 9. Heatmap of Knowledge and Skill Survey Responses for Quantitative Study**




### *Exploratory factor analysis*

Factor analysis aims to identify the underlying structure in a data matrix.[79] It is a statistical technique that transforms the correlations among a set of observed variables into smaller number of latent factors. It is useful for identifying groups of items which survey questions that are strongly correlated, we assume these groups of strongly correlated items represent some reflective factor. Factor analysis can be used to analyze whether the participant's responses on a certain set of items relate more closely to one another than to another construct.[80-84] It can broadly be divided into exploratory factor analysis (EFA) and confirmatory factor analysis (CFA). The **Figure 10** shows the model of factor analysis, observed item 1-6 can be measured in a test, they are modelled as linear combinations of the unobserved / latent factors, plus error terms ($\varepsilon_1$- $\varepsilon_6$). The item loading ($\lambda_1$- $\lambda_6$) is the magnitude of item-factor relationship, it represents how much item variance accounted for by factor.

**Figure 10. Factor Analysis Model**




Initially, an exploratory approach was adopted, in which the survey items derived from the qualitative findings and literature were tested. Exploratory factor analysis is a data-driven empirical exploration of the relationships among observed variables to identify the number of underlying factors that is not specified a priori. It can be used to elucidate how different items and constructs relate to one another and explore the dimensionality of the instrument.

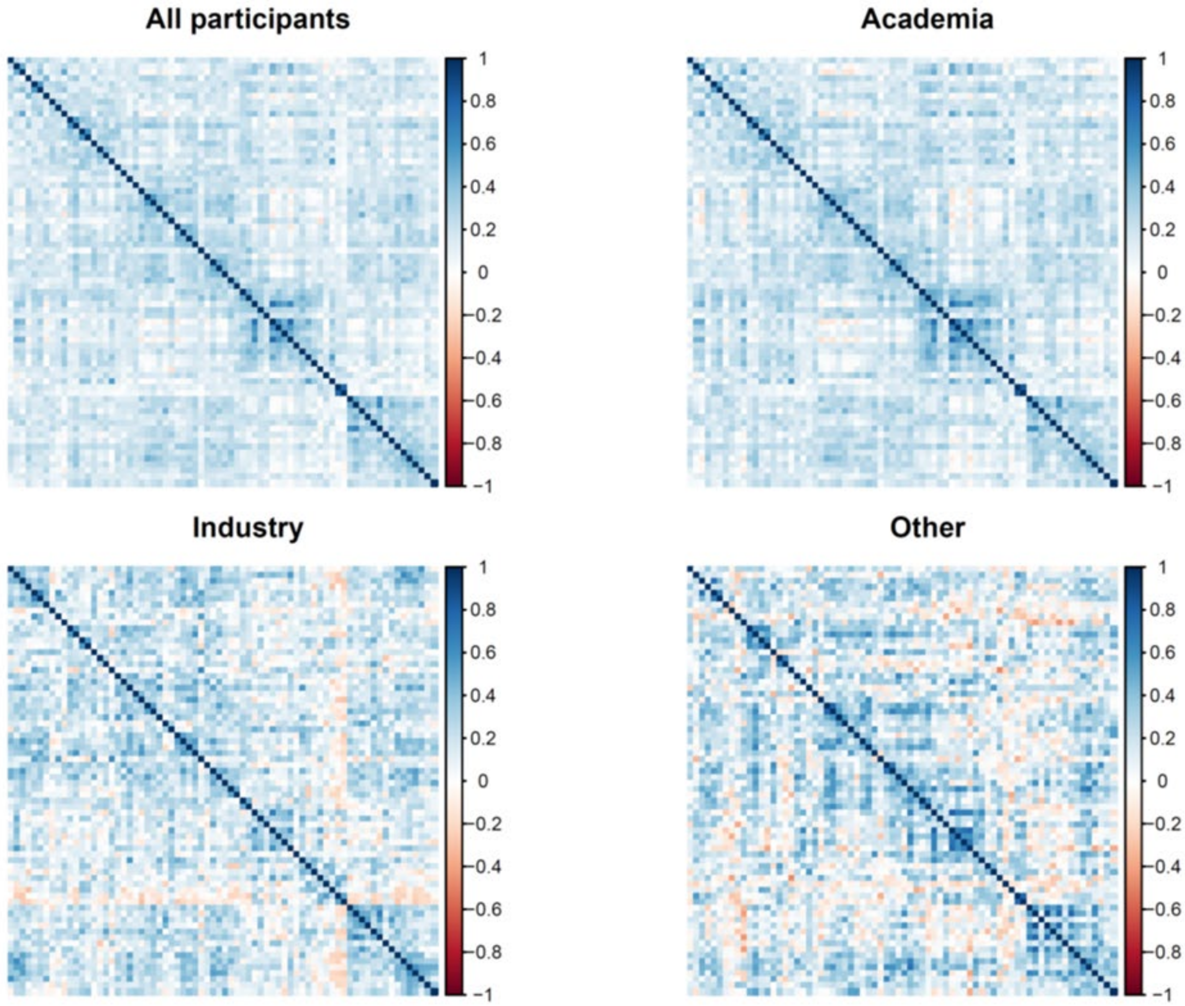
**Sample adequacy** The appropriate sample size needed for exploratory factor analysis is a multifaceted question. Larger sample sizes are generally better, as they will enhance the accuracy of estimates and increase statistical power[85]. The sample size needed depends on many elements, including number of factors, number of items per factor, size of factor loadings correlations between factors, reliability of the measurements, and the expected effect size of the parameters of interest[85-87]. For EFA, Leandre et al.[81] recommended that "under moderately" good conditions (communalities of 0.40–0.70 and at least three items for each factor), a sample of at least 200 should be sufficient, while under poor conditions (communalities lower than 0.40 and some factors with only two items for each factor), a sample size of at least 400 is needed. In this study, a total of 383 responses were collected, the observations was about five times of the variables and there are at least three items for each factor, thus the sample size was considered as adequate.

**Factorability** To be able to find factors within a data, there has to be at least a few sizeable correlations between individual items. Bartlett's test of sphericity can test whether the observed correlation matrix was identical matrix or not. It was used to determine if the data was suitable for factor analysis. From the results, $\chi^2$ (2556) = 12484.31, p value is less than 0.05, thus, the correlation matrix was not identity matrix. Therefore, it is appropriate to conduct factor analysis.

The correlation plot for all participants' responses on survey items was created to visually inspect the data that show the relationships to each other. The overall correlational structure of this dataset was checked. The interitem correlation matrix was coded to represent the magnitude of the correlation. In **Figure 11**, the darker shade of blue represents stronger positive correlations; the darker shade of red represents stronger negative correlations. The correlation plot can get a sense of how the items may relate to one another; the strong correlation may indicate that the items belong to the same factor.

The correlation plots for different job sectors were compared, the different patterns were shown in the figure. For academic faculty, items 1, 2, 3, 7, 33, and 55 had nearly no relationship with other items, but for industrial chemists, these items had positive or negative relationships with other items. It indicated that chemists in different job sectors may have different perceptions of the knowledge and skills that are required for their careers. It also may indicate that there would be different construct generated for each job sector.

**Figure 11. Correlation Plots for Participants in Different Job Sectors**




**Multicollinearity** For factor analysis, it is important that the variables not are too highly correlated (multicollinearity). Multicollinearity depends on two variables being too highly correlated (correlation >0.90) or too many moderately high correlations over a number of items (too many items with correlations > 0.70). If multicollinearity is indicated, one or several of the variables that are too highly correlated should preferably be deleted. In this dataset, there was no correlation coefficient was higher than 0.8, it indicated that there is no issue of multicollinearity in the data.

**Normality** Mardia's test is one commonly used test for checking multivariate normality. From the result of Mardia's multivariate normality test, the significant multivariate skewness or kurtosis values indicate multivariate non-normality.

| | Test | Statistic | p value | Result |
|---|---|---|---|---|
| 1 | Mardia Skewness | 71018.8389877347 | 0 | NO |
| 2 | Mardia Kurtosis | 97.3197429721312 | 0 | NO |
| 3 | MVN | <NA> | <NA> | NO |

Shapiro-Wilk test was conducted to check univariate normality for each survey item. The partial results were shown below, the p values indicate that univariate normality for each item was not met. It implies that robust estimation methods should be employed to handle non-normality in subsequent factor analyses.

| | Test | Variable | Statistic | p value | Normality |
|---|---|---|---|---|---|
| 1 | Shapiro-Wilk | x1 | 0.7540 | <0.001 | NO |
| 2 | Shapiro-Wilk | x2 | 0.7871 | <0.001 | NO |
| 3 | Shapiro-Wilk | x3 | 0.7614 | <0.001 | NO |
| 4 | Shapiro-Wilk | x4 | 0.8576 | <0.001 | NO |
| 5 | Shapiro-Wilk | x5 | 0.8231 | <0.001 | NO |
| 6 | Shapiro-Wilk | x6 | 0.4976 | <0.001 | NO |
| 7 | Shapiro-Wilk | x7 | 0.7364 | <0.001 | NO |
| 8 | Shapiro-Wilk | x8 | 0.7229 | <0.001 | NO |
| 9 | Shapiro-Wilk | x9 | 0.8469 | <0.001 | NO |

**Estimator selection** There are several different methods available, including unweighted least squares, generalized least squares, maximum likelihood, robust maximum likelihood, principal axis factoring, alpha factoring, and image factoring. One of the most commonly used methods for extracting variance when conducting an EFA on ordinal data with nonnormality is principal axis factoring[81]. Thus, it was selected for this factor analysis.

**Factor rotation** Factor rotation is a technical step to help interpret the output from the model[84]. There are two types of factor rotation: orthogonal or oblique.[81,84, 89] Orthogonal means that the factors are uncorrelated. Oblique allows the factors to correlate to one another. In educational studies, factors are likely to be correlated. Thus, oblique rotation was chosen for this data analysis. The previous studies also reported that the specific rotation method within the oblique category does not have a substantial effect on the results. The rotation method oblimin was chosen in this case.[90]

**Number of factors determination** An instrument that aims to measure one underlying construct is a unidimensional scale. The single total score can be used to represent the construct. However, the total score itself contains very little information about the intended construct. The multidimensional instrument was considered as appropriate in this study. Multidimensional scale should have at least three or more items for each subscale.

The commonly used criteria to determine the number of factors to extract were Kaiser's criterion[91], the scree test[92], the cumulative percentage of variance extracted[93], parallel analysis, and the most important, theoretical interpretability[94].

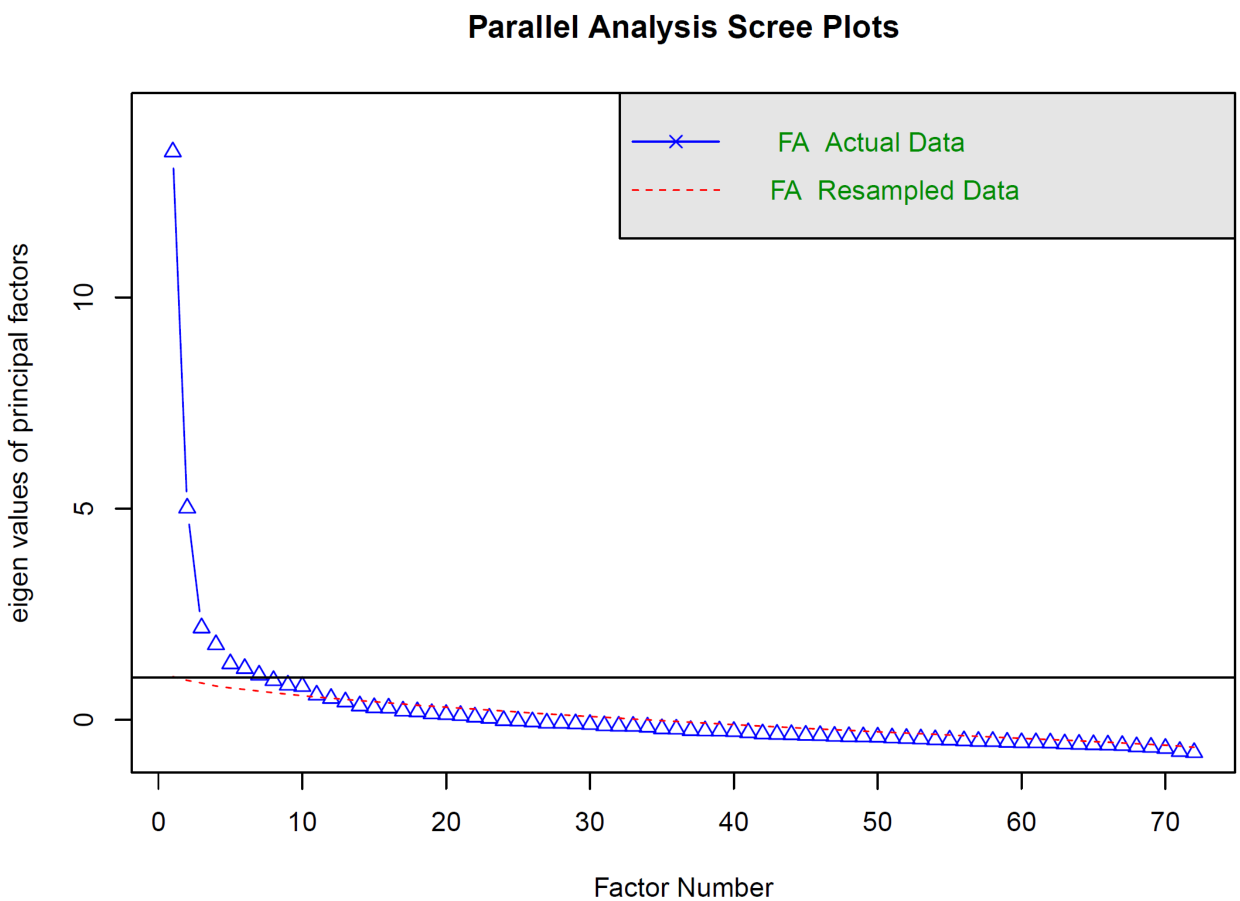
**Kaiser criterion** The number of factors is decided on the basis of the magnitude of the eigenvalues of the correlation matrix. The most well-known form of this criterion is Kaiser criterion, also known as K1. This criterion recommends that only factors with eigenvalues > 1 are retained, while factors with eigenvalues < 1 account for a small proportion of the variability in the dataset and generally do not add much information to the model[95]. Jolliffe[96] argued that this rule might be too severe and suggests a cut-off of 0.7, which has been used in a number of studies[97]. The previous study reported problems when using this criterion. The magnitude of eigenvalues is dependent on the number of items, and thus the sum of eigenvalues increases with numbers of items.[98]

**Scree tests** Another approach to decide the number of factors is the use of scree test[92], which aims to identify the point of inflection in a graph depicting the change of eigenvalues. The factors above the “elbow” are to be retained, the other ones are not. In contrast to Kaiser criteria, scree test is not affected by the number of items. The previous studies reported that the scree test works well at identifying the optimum number of factors in many research[99-100].

**Parallel analysis** Parallel analysis is the method that compares the eigenvalues obtained from the dataset to the eigenvalues generated from a simulated data to determine the optimum number of factors to be extracted. The Monte-Carlo simulated data are randomly generated based on the same sample size and number of variables as the actual data. This procedure also focuses on eigenvalues, eigenvalues are repeatedly calculated for this random data set. The eigenvalues generated from the simulated data represent the case that there are no real relationships between the variables in the dataset. Only those factors are to be retained whose eigenvalues exceed the average of the corresponding simulated eigenvalue.

In **Figure 12**, x axis is the factor number; y axis is the eigenvalue. these dotted lines represent the simulated data. We only are interested in the actual factors with eigenvalues that exceed the ones with the relationships between variables are simply due to chance. Principal components analysis is similar to factor analysis, but it is the analysis of the variance while factor analysis is the analysis of covariance, and thus principal components analysis usually yield a lower of components than factor analysis. This can give researchers a reasonable range of factors to retain. Based on these three types of criteria, the number of factors should be between 7 and 11.

**Figure 12. Parallel Analysis Scree Plot**




**Output interpretation** SS loadings are the sum of squared loadings. Generally, we consider factors worth saving if they have an SS loading greater than one. Proportion Var is the proportion of variance in the data explained by a particular factor. The higher this number, the more of the variance in the data it explains. Cross-loading describes an item that is influenced by more than one factor in the model. Cross-loadings with the difference below 0.2 are usually considered to be problematic. The factor loading results were shown in **Table 11**.

In order to determine the internal consistency of this construct, coefficient α and McDonald's omega were calculated. Coefficient alpha is the most used approach, but many studies reported that Cronbach's α underestimated the reliability of a test. McDonald's omega can provide information about the proportion of common construct value in a measurement relative to the amount of error. But, unlike coefficient alpha, McDonald's omega allows each item to be associated with the common construct influencing the true value of each item to a different degree. It was recommended as a more appropriate single-administration reliability coefficient than coefficient alpha. Both of them showed the good internal consistency of the instrument.

**Table 11. Factor Loading Results from Exploratory Factor Analysis**

| Item | Factor | | | | | | |
|---|---|---|---|---|---|---|---|
| | Factor1 | Factor2 | Factor3 | Factor4 | Factor5 | Factor6 | Factor7 |
| 45 | 0.88 | | | | | | |
| 48 | 0.85 | | | | | | |
| 42 | 0.72 | | | | | | |
| 46 | 0.62 | | | | | | |
| 2 | 0.59 | | | | | | |
| 3 | 0.57 | | | | | | |
| 47 | 0.44 | | | | | | |
| 10 | 0.39 | | | 0.36 | | | |
| 6 | 0.37 | | | | | | |
| 49 | 0.31 | | | | | | |
| 63 | | 0.81 | | | | | |
| 59 | | 0.77 | | | | | |
| 58 | | 0.62 | | | | | |
| 65 | | 0.50 | | | | | |
| 61 | | 0.50 | | | | | |
| 60 | | 0.42 | | | | | |
| 62 | | 0.41 | | | | | |
| 67 | | 0.37 | 0.30 | | | | |
| 69 | | 0.31 | 0.31 | | | | |
| 68 | | | 0.59 | | | | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 31 | | | 0.49 | | | | |
| 4 | | | 0.48 | | | | |
| 29 | | | 0.45 | | | | |
| 7 | | | 0.41 | | | | |
| 30 | | | 0.38 | | | | |
| 1 | | | 0.36 | | | | |
| 23 | | | 0.36 | | | | |
| 70 | | | 0.35 | | | | |
| 11 | | | 0.35 | | | | |
| 72 | | | 0.34 | 0.31 | | | |
| 12 | | | 0.34 | | | | |
| 66 | | | 0.32 | | | | |
| 64 | | | 0.32 | | | | |
| 14 | | | | 0.68 | | | |
| 13 | | | | 0.61 | | | |
| 18 | | | | 0.50 | | | |
| 55 | | | | 0.49 | | | |
| 17 | | | | 0.40 | | | |
| 16 | | | | 0.40 | 0.37 | | |
| 52 | | | | 0.40 | | | |
| 51 | 0.35 | | | 0.40 | | | |
| 54 | | | | 0.35 | | | |
| 41 | | | | | 0.55 | | |
| 36 | | | | | 0.52 | | |
| 15 | | | | | 0.52 | | |
| 35 | | | | | 0.50 | | |
| 33 | | | | | 0.46 | | |
| 34 | | | | | 0.43 | | |
| 39 | | | | | 0.43 | | |
| 37 | | | | | 0.37 | | |
| 20 | | | | | 0.33 | | |
| 40 | | | | | 0.31 | | |
| 28 | | | | | | 0.60 | |
| 38 | | | | | | 0.52 | |
| 24 | | | | | | 0.43 | |
| 43 | | | | | | 0.34 | |
| 44 | | | | | | 0.34 | |
| 21 | | | | | | 0.34 | |
| 26 | | | | | | 0.30 | |
| 56 | | | | | | | 0.80 |
| 57 | | | | | | | 0.75 |
| 5 | | | | | | | 0.31 |
| Coefficient α | 0.87 | 0.83 | 0.83 | 0.79 | 0.80 | 0.76 | 0.70 |
| McDonald's ω | 0.89 | 0.82 | 0.83 | 0.80 | 0.79 | 0.76 | 0.70 |
| Proportion Var | 0.07 | 0.06 | 0.06 | 0.06 | 0.06 | 0.04 | 0.03 |

| Cumulative var | 0.07 | 0.13 | 0.19 | 0.25 | 0.32 | 0.35 | 0.39 |
|---|---|---|---|---|---|---|---|

**Final solution interpretation** Once the factors and the items make empirical and theoretical sense, the factor solution can be interpreted. Based on the previous studies, each factor should contain at least three items. Therefore, there were seven factors retained in this dataset. The factor structure is shown below (**Figure 13**), each factor is labelled as one broad knowledge or skill category. Taking Factor 4 -- Research ability / technical knowledge & skills as an example. There were nine items loading onto this construct. The numbers shown in Table 11 were factor loadings. Factor loading explains how a given variable (survey item) relates to the different factors. A high factor loading suggests that the item is well explained by a particular factor. The items include:

develop existing technical skills (e.g. new methods) that I currently possess to some extent

acquire new technical skills (e.g. new methods) that I currently do not possess

systematically analyze quantitative data

analyze and interpret data related to my projects

identify solutions to the problems that have been identified related to the projects on which I typically work

identify problems related to the projects on which I typically work

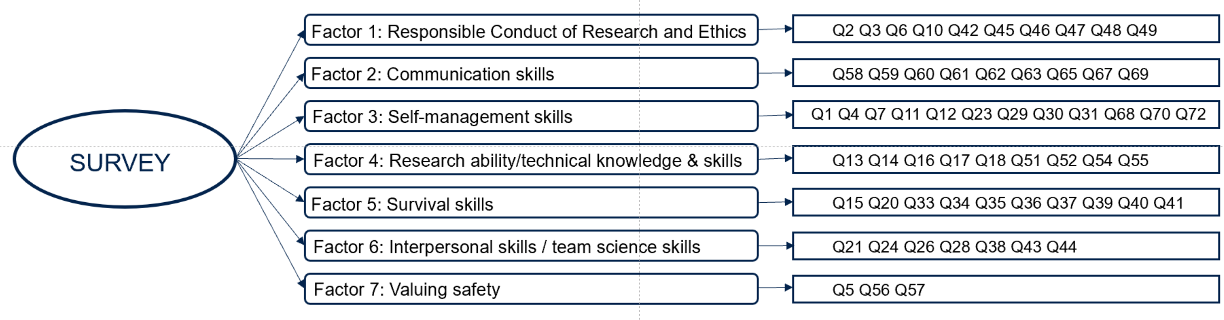
independently design and carry out projects

effectively search, retrieve, interpret, evaluate, and synthesize scientific literature

understand chemistry related to my projects fully

These variables had relatively strong association with the underlying variable, Factor 4. Based on the variables loading highly onto Factor 4, Factor 4 can be labelled as “research ability / technical knowledge & skills.”. Please see Appendix 10 for other factor interpretations.

**Figure 13. Factor Structure for Quantitative Study**




### *Confirmatory Factor Analysis*

Confirmatory Factor Analysis is used to determine to what the extent the data fits the previously proposed model. Essentially, CFA is to test whether or not the data collected can support the hypothesized model, which was derived from prior study. CFA is suitable when the proposed constructs are well interpreted and clearly articulated. The researcher can use CFA to confirm the hypothesized number of factors, the correlation between factors, and the relationship between factors and items.

The analysis of full survey used half of the data for exploratory factor analysis (EFA) and the other half for confirmatory factor analysis (CFA) to achieve the split-half reliability, which measures consistency between two halves of a construct measure. The criterions including root mean square error of approximation (RMSEA <0.08), comparative fit index (CFI>0.9), Tucker Lewis index (TLI>0.9), relative chi-square (.2 /df <3), standardized root mean square residual (SRMR =0.08) were used to assess the model fitness.

The indices indicate poor fit for our model. In this model, RMSEA is on the edge of cutoff 0.08, CFI<0.9, TLI<0.9, SRMR >0.08. Some studies did mention that factor structures obtained by EFA would turn out to fit poorly in CFA. In our case, the reason would be that there was a large proportion of items that had low correlation coefficient with one another.

### *One-way MANOVA*

After conducting exploratory factor analysis, these factors can be treated as new variables. One - way MANOVA was performed to compare the mean values of this new variable between job sectors. The Multivariate Analysis of Variance (MANOVA) is an analysis with two or more continuous response variables. The one-way MANOVA tests simultaneously statistical differences for multiple response variables by one grouping variables. The null hypothesis is that there is no overall difference in survey responses among job sectors; the alternative hypothesis is that there is overall difference in survey responses among job sectors.

The most commonly recommended multivariate statistic to use is Wilks' Lambda. However, Pillai's Trace was performed here as assumptions of MANOVA were violated. Pillai's Trace is more robust and is recommended when having unbalanced design. The statistics show that there was a statistically significant overall difference among the job sectors, $F(2, 379) = 20.736$, $p < 0.0001$. (**Table 12**)

**Table 12. One-Way MANOVA Results**

| | **Df** | **Pillai** | **approx F** | **num Df** | **den Df** | **Pr(>F)** | **Signif** |
|---|---|---|---|---|---|---|---|
| JobSector | 2 | 0.55919 | 20.736 | 14 | 748 | < 2.2e-16 | *** |
| Residuals | 379 | | | | | | |

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

### *One-way ANOVA*

Analysis of variance (ANOVA) test is to determine if the means of dependent variable (continuous) are different among independent groups (categorical/nominal) at one time. In order to identify the specific factors that contributed to the significant global effect, one-way ANOVA was investigated.

ANOVA with job sector as independent variable and broad knowledge or skill factor score as dependent variable was explored. Since the assumptions of ANOVA, which are normal distribution, equal variance in each group, and independent random sampled observations were not met, non-parametric alternative Kruskal-Wallis test was performed. (**Table 13**)

From the table we can see that there is a significant difference in Factor 1, 2, 5, 6 and 7 among job sectors. Note that, as there are seven dependent variables/factors, there is a substantial increase in type I error after multiple testing. Thus, we need to apply Bonferroni multiple testing correction by decreasing the level we declare statistical significance. This is done by dividing classic significant level (0.05) by the number of tests. This leads to a significance acceptance criteria of p value rather than 0.05. After the p value adjustment, Factor 5 and 7 no longer show the significant difference.

**Table 13. One-Way ANOVA Results**

| Factor | Effect | DFn | DFd | F | p | Signif | p.adj | Signif.adj |
|---|---|---|---|---|---|---|---|---|
| 1 | JobSector | 2 | 379 | 42.8 | 5.07e-10 | *** | 3.042e-9 | *** |
| 2 | JobSector | 2 | 379 | 4.67 | 9.68e-2 | | 1.936e-1 | |
| 3 | JobSector | 2 | 379 | 8.59 | 1.36e-2 | * | 5.44e-2 | |
| 4 | JobSector | 2 | 379 | 0.955 | 6.20e-1 | | 6.20e-1 | |
| 5 | JobSector | 2 | 379 | 28.6 | 6.07e-7 | *** | 3.035e-6 | *** |
| 6 | JobSector | 2 | 379 | 86.1 | 1.98e-19 | *** | 1.386e-18 | *** |
| 7 | JobSector | 2 | 379 | 8.14 | 1.71e-2 | * | 5.44e-2 | |

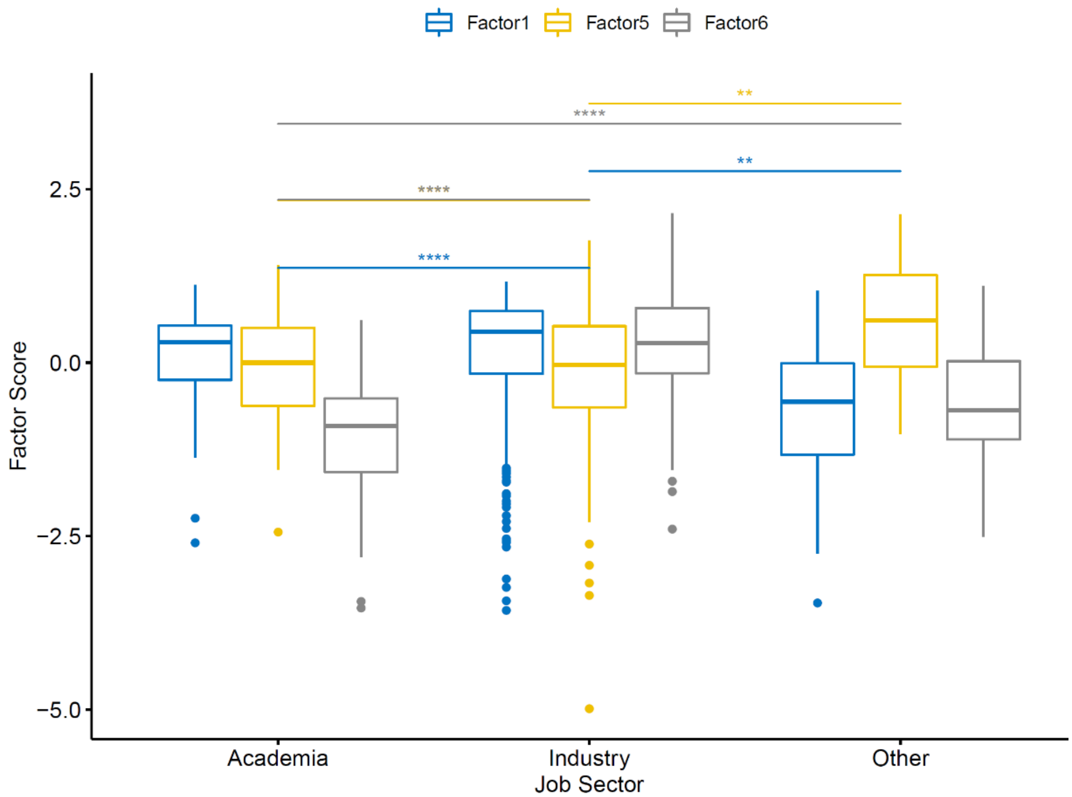
Signif. codes: 0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

***multiple pairwise comparisons***

A statistically significant univariate ANOVA can be followed up by multiple pairwise comparisons to determine which groups are different. Since the assumption was violated, Games-Howell post-hoc test was preferred. The boxplot in **Figure 14** grouped by job sectors, different colors represent different factors. After performing pairwise comparisons, some significant differences were shown on the plot.

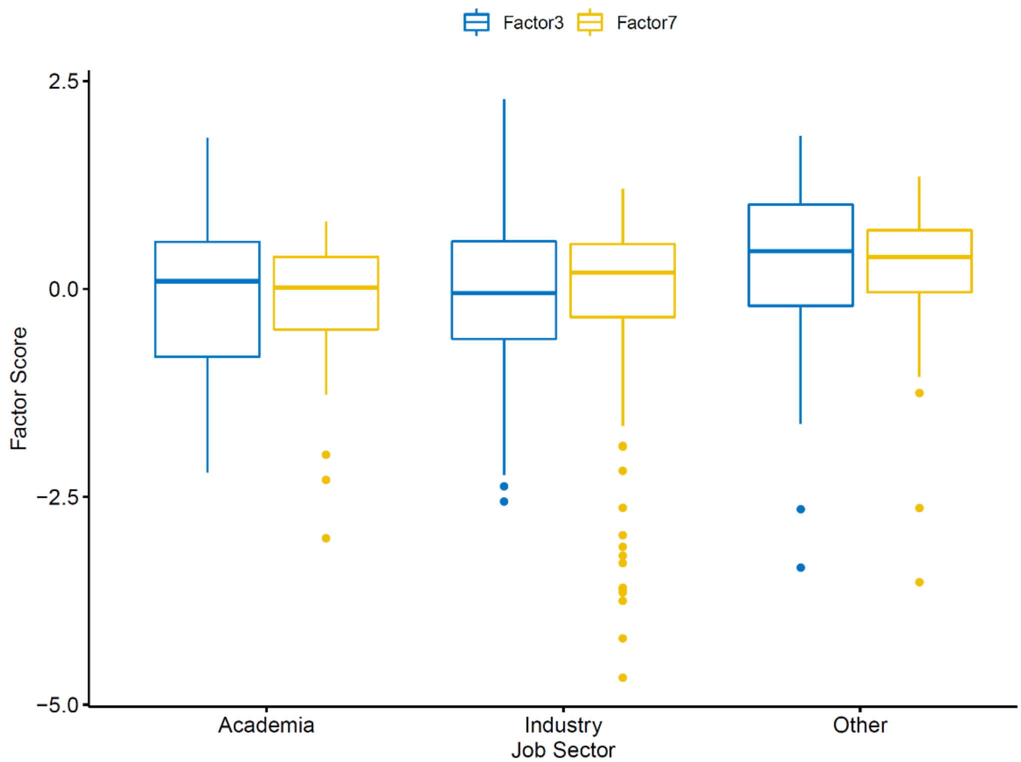
For Factor 1, industry is different from academia or other job sectors. The companies have their own organizational culture and work environment, they tend to have different requirements for employees compared to other job sectors. For Factor 5, industry is different from Academia or Other job sectors; Industry requires different general survival skills than chemists in another job sector. For Factor 6, academia is different from industry or other job sectors. We can get evidence from the previous qualitative research and some other studies to support the result. In chemistry department, academic faculty, especially research faculty tend to work on their own and do not emphasize too much on teamwork and interpersonal skills.

**Figure 14. Post-Hoc Test for Quantitative Study**




In Table 12, Factor 3 and Factor 7 were on the cutoff of the significant level. Due to its limitations of Bonferroni multiple testing correction, these two factors were also taken into consideration (**Figure 15**). They can provide weak evidence that chemists' perceptions of self-management and valuing safety were different across the job sectors.

**Figure 15. Pairwise Comparisons of Factor3 and Factor7 Across Job Sectors**


Factor3
Factor7
2.5
0.0
−2.5
−5.0
Factor Score
Academia
Industry
Other
Job Sector

# CHAPTER 4: LIMITATIONS AND CONCLUSIONS

## Limitations

For qualitative study, the research included voices from chemists in academia, industry and government, but there are a variety of other career paths that chemistry graduate students can take after graduation. While a healthy size for a qualitative study, our sample is not representative of all chemists nor do we claim that the results will be applicable in all situations. Our current analysis has also grouped all industrial members into three categories--R&D scientists, managers and consultants, which is an erroneous assumption as some of them take on more than one duty with diverse tasks. There may be an under-sampling of industrial chemists in non-technical roles or less technical roles, such as marketing and sales. Some chemistry career paths may not require chemistry expertise even though almost all in this sample did. Further research should expand the study to represent a diversity of voices from chemists in rich workplace settings.

For survey development, the sample size for this pilot study is 60, which is relatively small to run a factor analysis, especially there were 73 items in this survey, the data was high-dimensional compared to the number of observations. Literature suggested rules of thumb consisting either of minimum sample size in absolute numbers like 100 - 250, [71,72] 300,[73] or 500 or more[74] as reviewed by Dimitrov[75]. Another category of rules of thumb is ratio. In exploratory factor analysis, the sample size to variables ratio is used, the traditional rule of this ratio is 5:1. However, the sample size is even smaller than the number of variables in this pilot study. In addition, the assumptions of factor analysis were not met, leading the factor structure questionable. Therefore, those findings should be taken with caution. Future study should be conducted to investigate and compare some alternative approaches to fitting EFA in the case of small sample and high dimensional data.

For quantitative full study, the Likert-type scale used in the survey was treated as continuous variables, but the variables were ordinal variables as opposed to continuous variables. Furthermore, the survey responses distribution indicated a dominance of high ratings, leading multivariate and univariate non-normality in this dataset. Thus, the variables with log transformation or generalized latent variable models may help solve the potential issues. Additionally, Factor analysis is built on the analysis of the covariance matrix in the data and assumes linear relationships between items and between items and the factors, it has the limitation and suggests the use of non-linear factor analysis.

**Conclusions and implications**

The findings of the qualitative study in terms of knowledge and skills resemble similar outcomes of studies on *undergraduate* chemists.[28–30] While this indicates some overlap in requisite knowledge and skills between a bachelor and doctoral chemist, our results add additional details by showing the knowledge and skills that are emphasized in various sectors in the chemical sciences. Additionally, a plethora of research[34,46] dedicated to studying the transferrable skills that *doctoral students* need imply that doctoral chemists require a similar set of broad skills. However, the discipline-diverse sample makes these studies pose limited transferability to chemistry graduate education.

A number of observations can be made relating to how chemists discuss the required knowledge and skills for different job sectors. First, the majority of skills are required across both academic and non-academic careers. The results reveals that chemists will likely need much more than just technical knowledge and skills if they are to succeed in their careers. Second, in addition to the so-called “soft skills”, the themes in Figure 2 indicate what knowledge and skills play a key role in a chemist's daily tasks. At least a few chemists across all sectors reported that they needed the "soft skills" to succeed in their careers, but these soft skills are not traditionally emphasized in graduate programs.[1-2] Our results provide evidence that chemistry educators should be cognizant of the many knowledge and skills outside of traditional chemistry knowledge that influence success in diverse workplaces and the learning targets in traditional graduate programs can be misaligned with these required skills. The learning goals of graduate education should be more broadly as opposed to more narrowly focused. Our findings imply that if graduate programs wish for reform, they should provide more opportunities for students to develop skills such as communication, management, teamwork, and planning & organization. The American Chemical Society[2] and National Research Council[1] provide dozens of specific innovations for graduate programs, many of which increase focus on soft skills. Alternatively, faculty in chemistry doctoral programs can propose their own innovations via seminars, courses, informal retreats and individual mentoring to promote the skills highlighted by participants in our study.

Based on the findings of the qualitative study and previously reported studies, a 73-item online survey was developed. This study provided a detailed development process for survey development, it could be a good source for the development of a questionnaire. To date, empirical research on identifying knowledge and skills required by doctoral chemists has been limited. This survey measures doctoral chemists' perceptions of the knowledge and skills required for their careers. The results of this study provide support for the researchers and educators to better understand the construct of work competency.

The 12 broad categories generated from qualitative study derived an initial 73-item survey. Following a pilot test of the measure, a 72-item, nine factor solution was obtained. In this pilot study, the data indicated a dominance of high ratings, meaning that the participants required/valued most of the knowledge and skills in the survey list. After examining each item, item- understand my profession fully was deleted from the survey list; the item-foster group facilitation was modified to “foster good work climate and assist group members to accomplish tasks”. In addition, one factor generated from exploratory factor analysis was labeled as the miscellaneous factor, it indicated that these items were possibly on the drop list or needed to be rewritten. The final form of the instrument contains 72 items. The results of this study and the final factor structure support the notion that this instrument is a multidimensional construct.

The validity evidence was gathered in this study (evidence based on test content, response process, and internal structure). Factors had been identified that summarize the knowledge and skills needed by doctoral chemists from different job sectors. While from a developmental validity perspective, there is much work to be done gathering additional evidence with multiple samples, with this initial study has been well positioned to serve as a theory-based instrument to measure. The reliability evidence was collected in current study (evidence based on internal consistency and temporal stability). The test-retest reliability on total score level as well as item score level was calculated to show good temporal stability; coefficient alpha and item total correlation indicated the satisfied internal consistency of the construct.

This survey was distributed to a large population of chemists with doctorate in chemistry to achieve a national-level picture of the knowledge and skills required by chemists in different careers. The results show the evidence that doctoral chemists from different job sectors required / valued most of these identified knowledge and skills. and certain job sectors affect the way that chemists require and/or value certain knowledge and skills over other job sectors. For example, faculty in academia have different perceptions of teamwork and interpersonal skills over other job sectors. The study implies that the traditional learning targets in graduate programs can be misaligned with the skills required by chemists. Graduate students may benefit from a broader doctoral curriculum that would prepare them for a wide range of chemistry-related positions.

It is also notable that while the present sample of chemists from all sectors claims the importance of broad knowledge and skills such as communication and management skills, they tend to define and discuss them quite differently, thus supplying the most direct answer to the research questions. This implies that doctoral education is not one-size-fits-all even though it has been designed to be that way for over a century. Differences in how knowledge and skills are defined and perceived as necessary also indicate that doctoral education should be reasonably tailored to the individual students' career plan. This is because students on a specific career path may need a different set of subskills to succeed in careers within that path. Students considering career paths within academia and beyond may benefit from a broader doctoral curriculum or individual career development plans that would prepare them for a wide range of chemistry-related positions. In addition, developing co-curricular niche career exploration and skill development opportunities could support chemistry doctoral students. For example, student clubs, program/institutionally sponsored workshops, internships in careers of students' choice, and industry career training partnerships such as the NSF-funded Accelerate to Industry (A2i) immersion week program can help students develop professional skills and find satisfying careers.

In our sample, the industrial chemists generally focused on interpersonal dialogue and working in teams more frequently than either the research or teaching faculty in academia. This finding is well-supported by anecdotal conversations that lay out the differences between industry and academia as well as the general trend that industry works in teams on interdisciplinary projects. On the other hand, only a few chemistry research faculty discussed the necessity of knowing the audience when presenting, writing, or generally conversing. This is likely because the majority of research faculty interact with other research faculty, students, or generally other expert chemists, but this is not the case for industrial chemists who more often communicate with diverse audiences. Of particular interest and implication to chemistry departments is the importance of providing opportunities for graduate students to communicate with others outside of the chemistry department so as to build their skills in this area. For example, chemistry departments could invite guests from different disciplines to give departmental lectures or offer graduate students outreach to engage in public conversation. Additionally, doctoral students could implement recommendations from the American Chemical Society[2] and National Research Council[1] that develop interpersonal skills in courses outside of the chemistry department. Finally, graduate schools could provide more team experiences in classroom settings as the means to improve doctoral students' teamwork skills.

For best practice, chemistry graduate programs should explicitly target "soft" skills and professional development as core components. Specifically, chemistry departments can provide opportunities to graduate students to communicate science to a general audience and gain some other soft skills. Additionally, chemistry educators should make students be aware of existing professional society resources, such as ACS career portal, AAAS (American Association for the Advancement of Science) career trainings. They provide places for STEM or chemistry professionals to grow their careers with training opportunities, networking, and events. Furthermore, Dr. Branshaw and her colleagues in the University of Wisconsin, Maddison developed the Entering Research curriculum, which includes nearly 100 evidence-based activities for undergraduate and graduate research trainees to help them successfully navigate the research environment. In addition to these existing programs, chemistry departments can design some new programs to accommodate different career needs. For example, to better prepare students for their careers in industrial settings, grad students can learn project management, patent process, FDA regulations; for students who are interested in teaching positions, they can learn some teaching strategies, interpersonal skills form these professional development programs.

Cognitive apprenticeship theory is the traditionally assumed model for graduate education whereby a students' success is considered to be the product of their advisor's cognitive training. In this project, both qualitative study and quantitative study provide evidence that the cognitive skills are important for most of the doctoral chemists, and there is no significant difference existing between different career paths. The doctoral education goals as articulated in the literature were almost entirely through technical knowledge and the gaining of chemistry mastery with very little emphasis on "soft skills". However, the identified knowledge and skills in this study included "hard skills" as well as "soft skills" with the emphasis on "soft" ones. The results made us question the accuracy of the cognitive apprenticeship model.

Socialization provides a more wholistic view of how doctoral students might obtain knowledge and skills as they progress through chemistry graduate programs accounting for all sources of those knowledge and skills. It involves obtaining skills through explicit and implicit awareness of norms versus direct tutorial style instruction under cognitive apprenticeship. Socialization entails both cognitive and affective growth as opposed to a strict transfer of knowledge and skills from advisors to graduate students. The broad themes that were derived from qualitative study mostly came from the informal stage of socialization. The results in this study indicate that the knowledge and skills required for doctoral chemists' careers are obtained from formal and informal interactions, but not only cognitive training from their advisors.

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## Appendix 1: Interview Protocol

**Background Information**

1. Job title
2. Working years
3. PhD year
4. Research area

   (Industry categories: basic and applied research and development, analytical services, production, quality control, forensics, management, patents, licensing, trademark, marketing, regulatory, or training)

5. If industry: How big is your company? How many chemists do you work with?

**General questions**

1. Could you provide a brief description of your current job?
   a. What are your responsibilities?
   b. What do you do on a day-to-day basis?
2. In your opinion, what knowledge and skills do you need to successfully do your job?

   For each K&S:

   a. If you had to define ___________, how would you?
   b. Why do need ___________ to do your job? Can you provide an example?
   c. How does one gain ____________? What types of activities lead to its development?
3. In 2 or 3 sentences, could you summarize a research project that you've been working on recently?
   a. Briefly, where did this project come from?
   b. What are your responsibilities and the day-to-day activities that you do for the project?

c. What are some of the challenges you face in this project?

d. What knowledge and skills do you feel are necessary to overcome these challenges?

e. If you had to hire someone to replace you, what knowledge and skills do you think they need to have?

4. Out of the following, which knowledge and skill do you think is important for your career?

a. communication skills

b. teamwork skills

c. multitasking skills

d. teaching skills

e. time management skills

f. analytical and quantitative skills

g. writing skills

h. presentation skills

i. problem-solving skills

j. decision-making skills

k. networking skills

5. Before we conclude this interview, is there anything else about your experience influences how you are able to do your job that we have not yet had a chance to discuss?

End

- Thanks
- Gift card

## Appendix 2: Inter-Rater Reliability

```
> library(lpSolve)
> library(irr)
> DATA<-read.csv("IRR actual code.csv")
> data<-DATA[,6:8]
> kappam.fleiss(DATA2)
 Fleiss' Kappa for m Raters
 Subjects = 234
   Raters = 3
    Kappa = 0.8
        z = 129
  p-value = 0
> kappam.light(DATA2)
 Light's Kappa for m Raters
 Subjects = 234
   Raters = 3
    Kappa = 0.801
        z = NaN
  p-value = NaN
> DATA3mat <- as.matrix(DATA2)
> DATA3mat <- t(DATA3mat)
> DATA3mat
> kripp.alpha(DATA3mat)
 Krippendorff's alpha
 Subjects = 234
   Raters = 3
    alpha = 0.8
```

Four transcripts were coded for IRR, the transcripts and IRR codes are available for replication at DOI: 10.7910/DVN/VB2CBP

## Appendix 3: Code Book

open coding:

1. **Technical knowledge**: This refers to all information of hard skills, such as chemistry knowledge, experimental skill, literature evaluation, data analysis along the way, and previous working experience.

1.1 chemistry knowledge: This refers to both basic and advanced chemistry content knowledge; the need of PhD degree/background is also included in this code

1.1.1 basic chemistry content knowledge: basic chemistry book knowledge that every chemist should know

1.1.2 expert knowledge of chemistry: advanced chemistry knowledge in a certain chemistry field

1.2 experimental skill: This includes executing experiment, using instruments, collecting data

1.3 data analysis: This refers to all the information relating to data analysis

1.3.1 analyzing data: This includes performing data analysis to optimize the experimental conditions

1.3.1.1 forming alternative hypotheses: This includes considering if there is other potential explanation for the observation and run control measurement

1.3.1.2 designing experiment: analyzing data to help design experiment

1.3.1.3 multivariate data analysis: analyzing data as a function of multiple factors, it is useful for increasing yields

1.3.2 interpreting data: explaining results from instrument

1.3.3 quantitative analysis: This skill includes math and stat skills

1.3.3.1 mathematical thinking: This refers to calculation, solving equations

1.3.3.2 statistics: This is the skill for dealing with data that is generated from experiments

1.4 literature evaluation: This refers to literature searching, review and analysis

1.4.1 literature review: This includes the skill of reading papers, determining which need to be read in details and which can be skimmed through

1.4.1.1 read every detail

1.4.1.2 skim through the paper

1.4.2 literature searching: searching for scientific paper or patent literature for solving problems or getting research ideas

1.4.2.1 searching review article: searching one review article for basic concepts and steps, then get relevant papers

1.4.2.2 using different searching engines/database: This refers to searching by different engines/databases, such as Google Scholar, SciFinder....

1.4.2.3 patent literature searching: the ability to search patents

1.4.3 literature analysis: analyzing literature to identify research niche, evaluate the feasibility, formulate research question, propose solutions

1.5 relevant working experience: teaching faculty- teaching experience; research faculty-research experience; industry-working experience

1.6 computer literacy: This includes how to use Excel properly, coding, programming etc.

2. **Communication skill:** The abilities of giving and receiving different kinds of information

2.1 oral skill: This refers to any information about oral skills, via presentation or general talking without presentation

2.1.1 talking skill: general talking with people

2.1.1.1 interpersonal understanding: securing outcomes through interpersonal relationships, eg: having empathy, listening, sensitivity to others, being caring, awareness of other's feeling

2.1.1.2 know the audience: being aware of the technical or nontechnical audiences

2.1.1.3 clarify the purpose: This refers to the clarification of the expectations, purpose, topic of the conversation

2.1.1.4 effectively convey the idea: The ability to convey effectively, such as speaking clearly, conveying information clearly, knowing what should be spoken, knowing how to balance the conversation

2.1.2 presentation skill: This refers to oral skills via presentation

2.1.2.1 effective slides preparation: This refers to making nice and efficient slides and practicing before presentation

2.1.2.2 knowing the audience: knowing your audience who you will talk to

2.1.2.3 being organized: The ability to articulate the idea, clarify the purpose

2.1.2.4 speaking clearly: speaking clearly that other people can understand

2.1.2.5 time: being aware of presentation time, cannot be too long

2.2 written skill: This refers to any information about written skills, communication via written text, journals, books, grants, or other written materials.

2.2.1 organized: This includes articulating research idea and how to execute experiment

2.2.1.1 identifying logical route: knowing how to deal with details and find the most important aspect

2.2.1.2 outlining framework: outlining framework to get the idea

2.2.1.3 prioritizing: considering which should be written, written more or written first

2.2.2 writing clearly, explicitly: clarifying the significance, research objective, research approach, and explaining things in a way that reader can understand

2.2.3 concise: writing succinctly in a word economy way

2.2.4 meeting the requirement: meeting the requirement that can be the topic that readers are looking for, and the format of the written stuff

2.2.5 convincing: the written stuff is reasonable, novel

2.2.6 accurate: The information in written stuff is correct

2.2.6.1 grammar & spelling: paying attention to grammar & spelling in writing so that do not make reader feel confused

2.2.6.2 data: making sure data is accurate

2.2.7 knowing the audience: knowing who the reader is, inside or outside the field

2.2.8 practice and action: sitting down and putting words down

3. **Management skill**: The abilities that a manager, advisor, group leader should possess in order to fulfill specific tasks in an organization

3.1 lab management for research faculty: management skills used by research faculty in academia

3.1.1.1 supervising skill: This refers to giving students guidance and direction, and making sure they can meet the degree requirement

3.1.1.1.1 motivating students: encouraging students when they meet lots of failures or when they do not want to do something

3.1.1.1.2 advising students: giving students advice

3.1.1.1.3 assigning appropriate project: assigning different projects to different students based on their career goals and knowledge levels

3.1.1.1.4 providing feedback: giving students feedback after they provide the updates of their results

3.1.1.1.5 setting timeline: setting time table for students and monitor the progress

3.1.1.2 training students: This refers to teaching students new techniques, writing skills, or other knowledge and skills. Sometimes faculties may not teach directly, but students can learn from them.

3.1.1.3 securing funding: This includes securing external funding and keeping track on the budget

3.1.1.4 overseeing project: This refers to monitoring the project progress to make sure it runs smoothly in the proper timeline

3.1.1.5 organizing lab: This refers to making sure all equipment in lab is working, and organizing team

3.2 management skill for teaching faculty: management skills used by teaching faculty in academia

3.2.1 managing TA: This includes setting goals, training TAs to make sure they are well-prepared

3.2.1.1 training TA: The ability to train TAs for the labs

3.2.1.1.1 assessing TAs: evaluating TAs' work and providing feedback

3.2.1.1.2 giving orientation: making TAs know their jobs and responsibilities

3.2.1.2 setting goals: telling TAs the requirements and objectives

3.2.1.3 organizing lab: organizing meeting time and topic that need to be taught in lab

3.2.2 managing students: This refers to managing students in their classes or in labs

3.2.2.1 advising

3.2.2.1.1 advising available resources: being aware of the available campus resources

3.2.2.1.2 advising application process: advising undergraduates for graduate school application

3.2.2.1.3 advising writing: writing personal statement, CV

3.2.2.2 managing students in class

3.2.2.2.1 expectation

3.2.2.2.2 policy

3.2.2.2.3 syllabus

3.2.3 supervising lab manager: This includes training lab manager and setting standard procedures for them.

3.2.3.1 having standard procedure: having standard procedure that lab manager can follow

3.2.3.2 training: training lab mangers to make sure they do the job that they are supposed to do, including setting regular meetings and providing feedbacks

3.3 project management: The abilities to manage projects in industry

3.3.1 managing people: This refers to understanding what people need, require and accept, and managing them efficiently.

3.3.1.1 interpersonal understanding: the skills are used when communicating and interacting with other people, both individually and in groups.

3.3.1.1.1 respect people: the skills of showing respect to others

3.3.1.1.1.1 care about other’s time

3.3.1.1.1.2 listen to other’s opinion

3.3.1.1.2 motivating people: encouraging people to do what they do not want to do or overcoming their skepticism; understanding their goals and motivations

3.3.1.1.3 having empathy: seeing the world through other's eyes

3.3.1.2 making sure everyone knows their roles: making sure people know what they should do, and they suit a particular project or position

3.3.1.3 assessing the quality of work: evaluating people's work to see if they meet the goals both for company and themselves and if they make mistakes and giving feedbacks

3.3.2 managing time: This refers to figuring out what needs to be done in what order and how quickly it can be.

3.3.2.1 establish timeline for the project

3.3.2.2 balancing time: balance time for multiple projects

3.3.2.2.1 being flexible: being flexible to keep things move forward but accommodate with the plan

3.3.2.2.2 balancing time for multiple stakeholders

3.3.2.3 knowing when to quit: when the project cannot move on, know when to stop it

3.3.3 setting goals: This includes knowing the objective and the mission of a project.

3.3.4 managing budget: This includes knowing the cost, resources, sponsors, and keeping an eye on how money has been spent.

3.3.5 patent management: This refers to management of patents and intellectual property.

3.3.5.1 knowing the patents: knowing what the patent is, the types of patents and when is the right time to file a patent

3.3.5.2 understanding patent system: knowing how the patent system run

3.3.5.3 helping with patent writing: the ability to write patent or help writing patent

3.3.5.3.1 translation: translate notebook reaper to patent examples

3.3.5.3.2 understanding patent claims: understand what are the patent claims and what is the purpose, how to include as much as possible

3.3.6 risk and uncertainty management: This refers to reducing risk and uncertainty of a project.

4. **Teamwork/collaboration skill**: This refers to all the skills needed in working with others

4.1 interpersonal understanding

4.1.1 being open to other's idea: being willing to listen to others' opinion, to accept different voices, to be a good listener, to be flexible for different thinking ways

4.1.2 being persuasive: persuading someone to do or believe something through reasoning

4.1.3 caring about others: treating people nicely, recognizing the best way for different people

4.1.4 motivating collaborator: giving collaborator encouragement

4.1.5 trusting collaborator: appreciating collaborator's idea, and trusting them

4.2 sharing learnings and experiences: sharing what have been learned from the previous project and take to the next one

4.3 whom to work with: classifying different kinds of collaborators

4.3.1 co-workers with different expertise: mostly are the collaborator in the same department/discipline, but having different expertise, such as biochem & p-chem; biochem & electrochem

4.3.2 group members: collaboration within the same group/team

4.3.3 interdisciplinary collaboration: collaboration between different disciplines, like chemistry and biology, chemistry and physics

4.3.4 other experts in similar field: collaborators in the same area but in other college/university/organization

4.4 having a scope: knowing the team goal, rules

4.5 everyone knows the progress: allowing people who have done the job to see the result and conclusion

4.6 giving feedback: providing feedback to collaborators

5. **Planning & organizational skill**: The ability to organize oneself & others; manage time; organize tasks

5.1 time management skill: These are the methods to manage time better

5.1.1 balancing different duties: balancing time to find what is necessary

5.1.2 blocking certain time for certain thing

5.1.3 planning ahead: having a to-do list, planning in advance. In industry it always means establishing a timeline

5.1.4 prioritizing: identifying the most important thing and spending time on that

5.1.5 thinking back: analyzing what had been done today

5.1.6 being flexible: being flexible with unexpected things

5.2 organizational skill: the ability to organize oneself and others

6. **Teaching skill**: the abilities to teach other people

6.1 course preparation: This refers to preparation of a course, including preparing lectures, homeworks, exams, labs etc.

6.1.1 how to use chemistry: teaching students how chemistry can be used or the relation to the real world

6.1.2 knowing available resources to students: telling students what the available resources for them are, textbook, online resources etc.

6.1.3 learning materials meet experiment requirement: making sure the classes are associated/aligned with labs so that students can understand better

6.1.4 lecture, questions, exams, homeworks preparation

6.1.5 prioritizing topics: identifying the topics that are the most important

6.1.6 using equipments/instruments: equipment includes running laptop; instruments are for both general chemistry & upper level chemistry courses; including demonstration

6.2 teaching strategy: This refers to all the teaching strategies that can help student learn better

6.2.1 doing a lot of practice: assigning a lot of practice to students in order to make them be familiar with the information

6.2.2 giving examples: after teaching concepts, giving students example so that help them have a better understanding of the concepts

6.2.3 preparing pre-class questions: preparing pre-class questions to get students learn ahead

6.3 learning from other sources: learning from Internet materials & learning from other universities

6.3.1 learning from journals: reading papers and learning from journals, such as CE, JCE

6.3.2 learning from online resources: This refers to all the online resources beyond journals and textbooks, such as Youtube video, online program

6.3.3 learning from other university: learning the methodology that can be improved in other university

6.4 explaining in simple terms: breaking concept down in simple words

6.5 interpersonal skill: this refers to listening, approachable, awareness of other's feeling, caring

6.6 being responsive: This refers to both asking questions and answering questions, and responding quickly

6.6.1 answering questions: This refers to all the approaches of answering students' questions

6.6.1.1 email responses: answering questions via emails

6.6.1.2 holding office hour: holding office hour for answering students' questions

6.6.2 asking questions: This refers to all approaches of asking questions, inside and outside class

7. **Personal value/attributes**: the combination of characteristics or qualities that form an individual's distinctive character, such as knowing how to read people, how to influence people, having a sense of humor, positive work attitude, work ethic, impact & influence on others, high Emotional Quotient etc.

8. **Problem solving skill**: the ability to find solutions and handle difficult or unexpected situations.

8.1 problem solving in class: solve problems on the textbook

8.2 trouble shooting: problem solving beyond the textbook; including troubleshooting technical problem and general problem solving

8.2.1 general problems: solve general problems in life

8.2.2 technical problem: solve technique/research problems

9. **Personal growth/development**: This includes the willingness of learning new things and keeping practicing after learning, openness to feedback, having developmental insight

9.1 being willing to learn new things: being curious and willing to learn new things and searching for new opportunities

9.2 taking class/training: being willing to take classes or trainings to develop knowledge and skills

9.3 keeping practicing after training

10. **Critical thinking**: The abilities of making reasoned judgments that are logical and well-thought out

10.1 creativity: being innovative for problem solving and getting research ideas

10.2 connecting small pieces: being able to connect dots that are accomplished, linking skill

10.3 being aware of external influences: being aware of external resources rather than things in the lab

11. **Organizational awareness**: This refers to improving awareness and identity, developing talents and potential, building human capital and facilitating employability, enhancing the quality of life and contributing to the realization of dreams and aspirations.

    11.1 business mindedness: This is the skill just for industry people, knowing cost, capital and how company make profits

    11.2 understanding rules and regulations: understanding and adhering to the rules and regulations

12. **Networking skill**: making positive impression on other experts, be willing to advertise yourself and establish reputation

## Appendix 4: Transcripts Examples for Qualitative Study

**Example 1**

Date: 01302018 KS1

Interviewer: Alright so we are now recording here if you can just state one more time for the record that you are okay with being recorded.

1: Yes, I'm okay with being recorded.

Interviewer: Alright, appreciate that. So do you have any meetings coming up here in the next half an hour?

1: No, I'm all free, available for the interview.

Interviewer: Great, thank you. Okay, so we found you are an assistant professor at [university], is that correct?

1: Correct.

Interviewer: Correct, and what year did you get your PhD?

1: 2010.

Interviewer: 2010 and then what would you say is your research area in chemistry?

1: Bioanalytical chemistry.

Interviewer: Bioanalytical?

1: Yep.

Interviewer: Okay, so could you just provide a brief description of your current jobs? Like what are your responsibilities, what are your day-to-day activities in your role as an assistant professor?

1: Okay. I'll describe my job responsibility maybe splitting in terms of percentage: maybe 60% for research, 30% for teaching and 10% for service. So the research would include supervise students and extract external funding and establish external funded research. Teaching would include teach undergraduate level and graduate level classes and service would be provide service to the college and the university as well as the department.

Interviewer: Okay. Thinking about that research requirement you are talking about, supervising graduate students and then securing funding. I'm thinking about supervising graduate students, what kind of knowledge and skills right after that do you feel are necessary in order to do that?

1: I would say definitely the first of all the technical skills are required. Those trainings I learned from the PhD and postdoc experience. And I would say many of the things I learned in terms of supervising, really supervising and teaching student, I learned from postdoctoral experience in terms of how to run a lab, how to, say, manage a lab and then assign appropriate projects to the students, and then oversee their project progress and advising them along the way, including help students troubleshoot, things like that.

Interviewer: Okay, kind of looking into more of this supervision and management role if you haven't defined the management skill, how would you define management? What types of things are consumed in there?

1: I would say in terms of keeping students on track, remind them, motivate students and encourage them to pursue a specific research or a career goal, and setting a timeline for students and then occasionally or maintaining a schedule, keeping them on track and then receive updates from students and providing advice and then maybe provide necessary feedback for them to make sure they are on track and then making necessary progress towards their goal as well.

Interviewer: Okay. So kind of making sure they are on track, motivating them and encouraging them and said at the beginning specifically for their career goal, correct?

1: Correct.

Interviewer: Okay. For providing feedback specifically, you know, why is that necessary for this particular part of your job?

1: I think I'm the main person they are relying on when doing research. And if I have certain requirement for doing a project, and they go there to perform certain experiment themselves. And then when they bring back results to me, they think it's necessary for me to help them double check the results, and they also make sure they are correctly interpreting the results, and then whether they are on the right track designing the next experiment, and to make sure they are on track in terms of completing the project as well as learning the necessary skills for their training per se.

Interviewer: Okay, and then you had mentioned some technical skills previously, can you briefly describe some of those technical skills? Not necessarily the specific techniques, but you know what would be included in that?

1: So based on the nature of the research were conducting right now, I would consider the quantitative analysis to be an important part that I learned in my training, to carefully execute experiment, to critical analyzing the results, and also at the same time review literature and to put our results in the context, and then carefully and kind of interpret our findings, and then try to extract the significance out of it.

Interviewer: Okay, so this is still kind of a little, I know it's a very broad topic of quantitative analysis, you talked about the process of results, reviewing the literature, interpreting all findings kind of appropriately. Can you break down any more specific skills or knowledge that would be required for each of those components or all process as a whole?

1: I think one of the components is the mathematical skill. We do a lot of the enzyme kinetic analysis. I think that requires certain mathematical background. That's one of those. And I think second of all is to involve some of the statistics skills in terms of analyzing the data as a whole, and to put all of the data in a certain context, and then interpreted data correctly.

Interviewer: Okay, and then real briefly could you talk about mathematical and statistical skills? Could you give me an example of each of those?

1: So mathematical skill is more of doing routine calculations, so for a simple example, like how to prepare a buffer, how to calculate the buffer components. And statistical skill is, for example, when we have a set of data with seven or eight numbers, how to do for example student t-test and to effectively eliminate potential outliers, and then calculate the standard deviation things like that.

Interviewer: OK, and then heading back up we switch over from the supervisory role that we've been talking about, another big thing that you had mentioned in the research component of your job was securing external funding and kind of establishing a program like that. What types of knowledge and skills do you feel like would be necessary in that aspect of your career?

1: So are you talking about for a training perspective, what kind of knowledge of skills we should prepare students? Early on their career?

Interviewer: Strictly for you, what knowledge and skills do you feel like you use and secure funding for your own research program?

1: I think doing literature analysis, that's important one. And second of all, I think the writing skill is another very important component.

Interviewer: Okay, and that first one is doing the original analysis?

1: The literature analysis.

Interviewer: Literature analysis, I'm sorry. And then in conducting that literature analysis, can you break down like what are you looking for in typical literature analysis? What types of skills do you need in order to conduct a good literature analysis?

1: I'll say we have to be critical in analyzing certain area, and then be able to search the current literature and critical analyzing the current state of art of that specific research area. And be able to identify a research niche, and then also evaluate the feasibility of doing that type of research in this research environment that the PI is positioning. And lastly be able to summarize the whole thing and formulate into a research question and then propose a solution that is achievable.

Interviewer: Okay, and sounded like there might have been some overlap the other big skill you mentioned was the writing component and the writing skills, so there might be some overlap within writing a research question and that kind of thing. Can you elaborate any bit about what kind of skills are included in this kind of umbrella writing skills?

1: Yeah. So the writing skill I considered the logic of organizing the proposal is the important first step, and then identifying the research question as we already did in the literature analysis. But it's specific for writing, we will be able to formulate in a logical way to clearly, explicitly state those components like significance, research objectives, and align the necessary research approach that can address that specific problem we identified, and then write a convincing research proposal that we will get it funded.

Interviewer: Okay. And then I think you kind of mentioned this, but some of the things we've just been talking about here, how do you go about gaining those knowledge and skills? You talked about your graduate work, your postdoctoral experiences, were those the main sources for the skill development?

1: I will say perhaps many of those skills I learned on the job. I did have some experience, reading some previous successful proposals from my PhD and then postdoctoral adviser. But I think until I did it myself, writing my own research proposals that I learned the most I would say.

Interviewer: OK. And then does that also apply for supervising and managing your research group? Is that kind of an on-the-job thing as well, or you feel like that was more for a graduate school and postdoc work?

1: More for graduate school and postdoc.

Interviewer: Okay. So I may kind of change gears here just a little bit, instead of asking kind of on a whole of your job, we are gonna focus just on a real quick recent project that you have been working on. So can you think about the recent project that you have been working on, and in about two or three sentences just give me a summary of a recent research project that you have been working on.

1: Okay, so one of the recent research project we are working on is to really look at the catalytic details of an enzyme. This enzyme is a normal DNA polymerase, and then basically copies the DNA. And then we are trying to use biochemical and structural biology approaches to study the kinetic details of this enzyme in terms of catalysis. And I'm doing kinetic analysis specifically.

Interviewer: Okay, so looking more towards the kinetics of it.

1: Yep.

Interviewer: Kind of where did this project come from? Was this your own independent project? Is this collaboration or?

1: Yeah, this is my only independent project.

Interviewer: Own independent, sure. What are your responsibilities in the project and kind of what your day-to-day activities look like in relation to this project?

1: I would monitor progress, I would oversee the whole project, and then doing necessarily research, and supervise students of course, students and postdocs, and to oversee their progress, offer feedbacks and then summarize the data and perhaps having meetings with students and postdoc to help them organize the data and then put together publications.

Interviewer: Okay, so look like a lot of it was towards the kind of monitoring, overseeing, managing and that sort of thing, and we've already talked about that a little bit. Have you been in the lab to do research yourself? It's completely fine if you haven't.

1: I did work in the lab occasionally, but not specific on this project recently.

Interviewer: Okay. So what kind of challenges do you face in some of these day-to-day activities with this project?

1: Perhaps finding more time to do certain things. Struggle around among different jobs and try to balance everything, prioritize things and always find the right thing to do at the specific moment.

Interviewer: Okay. When it comes to that balancing, prioritizing time, do you have maybe general suggestions or even a specific example of how you are going to choose to balance and prioritize time or a particular experiment or something like that?

1: If we are talking about specific experiment, definitely keep eye on the corner research and see what potential competitors are doing. And if the certain aspect research is already done in the field, and if that's the case, quickly switch or find new opportunities for that project. And in terms of the time management, I think everybody is familiar with the 80/20 rule, and then try to find the most important thing and also identify the not-so-important thing, for something's deadline comes close, and then tried to allocate my most precious time. I'm a morning person, so I’d like to spend the most precious time on the most important thing in the morning, and then maybe in the afternoon when I'm getting tired, I will spend on other things that's not so important, but I just have to get it done.

Interviewer: Okay, particularly with kind of two big things, there was identifying the potential competitors I think you are talking about, other people doing similar research. What knowledge and skills do you feel like they are required to identify those competitors and that type of thing?

1: I think that the literature search would be enough, and usually assembly doing good literature research either on Google or PubMed, usually those similar recent topics will pop up, and then spend time analyzing those existing researches, and then it's not too difficult to identify competitors.

Interviewer: Okay, and it might seem a little redundant with what we were talking about previously, but can you break down the ability to do a literature search into more specific skills or knowledge like what does it take to do a good literature search?

1: I would say try searching different keywords and of course you use different search engines, maybe try also some of the public database, funding database like NIH report or on the NSF website on those funded research projects, or any public available information like the DOE or DOD, try to find available project that's already funded, and see if there are identified potential competitors or people are doing similar research besides research papers.

Interviewer: Okay, thank you. You also mentioned the time management that come up a couple of times. Ultimately how do you manage the time? Like what are the big skills and knowledge that you need to keep yourself in check and knowing which projects and which experiments to prioritize? Again, that might seem a little redundant with what we were talking about previously.

1: I think it's important to establish a to-do list, maybe weekly or even daily, right? So what are the things I want to accomplish this week or today, and keep that checklist and then identify the most important thing on the list and then get it done sooner than later. And then perhaps again just keep a certain block of time working on certain things, and designate certain time working on certain things, and then protect that time to do the most important thing.

Interviewer: Specifically within this project of looking at the kinetics of this enzyme that you are looking at, can you think about a specific meeting that you have had with a graduate student or one of your postdocs, and just tell me about that meeting a little bit, related to this project about where you provided your oversight and feedback to the project?

1: Okay. So I'm actually running this weekly meeting with a lot of my lab members. So for them to provide research update, and for me to provide feedback to them. So a typical meeting would be that a student and I will look at the data they obtain the past week together, and so they will use a few PowerPoint slides to summarize their data in the past week. So I would ask them to interpret the data for me first, and then if suggestion needs to be made, I will comment on those and provide feedbacks. And then I would also encourage them to summarize their data in the past week, and then make plans for the following week, and then make that logic connection between the previous and next experiment. And then ask them what is the reasonable timeline to accomplish those experiment, and help them set a goal. So both summarizing the previous week and to make plans for the following week or weeks.

Interviewer: OK. I mean the last relating to this specific project, if you have to hire someone to replace you, what knowledge and skills do you think they would need to have?

1: If you are talking about technical skills, I would say the main mechanistic entomology skills would be necessary to accomplish this project. And other non-technical skill, I would say some things like people typically do, like time management, efficient and productive PI, and someone also be able to supervise students, and then provide feedback and provide necessary training for students.

Interviewer: Okay, and the second thing you had mentioned some about end product was that towards the quality or just trying to get to the end product?

1: Just trying to get the end product.

Interviewer: Got you. Okay, moving in the last little section about the interview. Sorry I think we got about another 5-10 minutes, is that okay with you?

1: Okay, yeah.

Interviewer: So instead of not asking about a specific project, I'm just gonna kind of list a couple of skills, and I'd love to just hear your comments on which you think is important for your specific job and any comments you might have about each one of them. So can you talk about communication skills? You feel like that one is important for your career?

1: Yeah I think that's important. I think I forgot to mention it in several different context in our previous question. During a student training, during our weekly meeting, I asked them to present their data logically, at first I would offer a feedback if certain correction needs to be made. We also have regular group meetings that students presented their data. Usually I provide necessary feedbacks to organize a nice and logical presentation. So I also emphasized the difference between a poster presentation format and our presentation format, so in a different context. So I think communication for both oral and writing communication, I think those are critical for this job.

Interviewer: And in your role as an assistant professor, do you think team working skills would be valuable in your career?

1: Yeah, absolutely. I think both in a research team, having that team spirit, build it into the group, encourage student to collaborate and help each other. And then also on top of that, for myself, in terms of finding necessary collaborators or finding people with similar interest, and then to develop network and having a network of people either to collaborate directly or just share a bunch of ideas, I think that's a very important skill.

Interviewer: Okay, and then the next would be teaching skills. This is specifically within the context of your research proportion of your job, not the teaching portion, do you think that teaching skills are important in the research portion of your job?

1: I think so, right. So because the training of students, and this really depends on the teaching skills, say if I want to explain a problem or a concept to students, right? Or show students the right way to present something, right? So I think that logic is quite common when you are presenting a research topic or presenting a teaching topic, right? So I think this is important.

Interviewer: Sure. Potentially related would be presentation skills, do you feel like that's important for your role as an assistant professor?

1: Yep. I think a lot of time that the assistant professor is being invited to some other institution to present their research. I think this is a good way to advocate my research or made by myself known in a field. And presentation skill I think is a part in the writing as well, in terms of how to organize the project and organize research problem, and try to promote it to a review panel per se.

Interviewer: Okay. How about general problem-solving skills?

1: I think that's also important. Although a lot of time it's hard to define clearly, but I think that's also important.

Interviewer: Give me an example where you might have used problem-solving skills or needed problem-solving skills to work through something?

1: So a lot of time we have to do this troubleshooting when we establish a new procedure or a new experiment. So problem solving I think comes in a big part in helping us to troubleshoot or clarify some of the procedures or just make a procedure feasible in our hand.

Interviewer: Okay, and then when you are saying troubleshooting there, you're not just referring to like when an instrument doesn't work, you are talking about like an experiment isn't working or something?

1: Yes. Most of the time I'm not talking about the technical difficulties in the instrument, but most of the time is about finding the reason that the result is not as we expected or find the right solution for a few experiments per se.

Interviewer: Okay, thank you for that clarification. Two more for you here, decision-making skills, you feel like that's required for your role?

1: Yes, in particular when overseeing a big project, in identifying the most important thing to do at the moment, or also try to find a right student to accomplish certain experiment.

Interviewer: Okay, so identifying the right person for the job as well as identifying the most important experiments to focus on.

1: Correct.

Interviewer: The last one would be networking skills.

1: I think this is perhaps particularly important for a new PI. Because oftentimes that we need to make our work known to the colleagues in the field, right? So that networking skill is important in achieving that, right? So either in a conference or more informally in other venues, right? So the other type of symposium either locally or nationally, so I think it's important especially for new PIs.

Interviewer: Okay, anything generically about the last half hour of conversation that we've had here, is there anything else about your experience as an assistant professor that there's a certain knowledge or skill that enables you to do your job and you don't think that you wouldn't be able to do without it?

1: There are so many of them, but it's really coming as a package. So I would say it’s hard to identify one. I think if I were to identify one, I'll say the time management perhaps, this is a true for assistant professor, this is true for every job if you want to do it well. So time management I would say that's the key to be successful.

Interviewer: Okay. Well, thank you again very much. That's all I had for you. We really do want to use these responses to help change graduate school and improve PhD preparation of students. We're happy to give you gift card for participating in this interview today.

**Example 2**

Date: 03052018 KS21

Interviewer: Do you have anything coming up in the next half an hour or so?

21: Nope.

Interviewer: Okay, and then I will try to keep you to that half an hour. If we need to go a little longer, we'll make sure to ask for your permission. So let's just start real quick with your job title. What is your official title?

21: Senior scientist.

Interviewer: Senior scientist, and how long have you been at [company]

21: For 10 months.

Interviewer: For 10 months?

21: Yep.

Interviewer: Okay, and what year did you get your PhD?

21: 2009.

Interviewer: 2009, and out of the five kinds of traditional research areas: biochem, p-chem, what do you feel like this job has you doing most of?

21: My new job is a little bit more microbiology actually than anything else that I've done. So prior to that I would say it was protein chemistry.

Interviewer: Okay, protein chemistry, definitely in the biochemistry kind of area.

21: Yep.

Interviewer: And then what kind of industrial category would you kind of classify your job? You know, things like basic and applied research and development, analytical services, production quality control, those types of things?

21: It's really quite in the middle of all that actually. The group that I'm in right now is called BPS, which is bioprocess science, and this group is responsible for transferring new processes from R&D to manufacturing, and that includes a lot of coordination with QC, and other department. But then the other element is that as processes are run for years, and they start to have issues. Those processes come back into our group, and so it's all about understanding increasing and decreasing air. What's related to that is the raw materials, is the process, is the test that's changed. So it's really kind of a mix, to be honest.

Interviewer: Okay. And then generally do you know how big your company is? In particular, how many chemists or you know scientists you work with?

21: So I am in a group of 30. About 30, 28 or so. The larger R&D organization on this site is just to 100, total in my group. I don't know the global, may be 1400.

Interviewer: 1400.

21: Yes, that's global.

Interviewer: All right, thank you. So we're gonna hop right into the first set of questions here, which is just a very broad kind of what do you do on a day to day basis? What are your responsibilities? And just kind of what is the brief description of your job?

21: So my job is for downstream processing, it related to elements of formulation. So I work with the product mainly after it's gone through any downstream concentration, and work to ensure that we have good presentations' ability. So that might include development of excipient soar stability parameters for a new product, or like I'm working on person existing products troubleshooting to understand what element of causation or formulation is causing a decrease in potency.

Interviewer: Okay, specifically when it comes to those developing the parameters, and what kind of parameters were you looking at again?

21: So right now we look at different elements of stability and in the animal health space the products are not higher purified. So we use a lot of different methods and you wouldn't do for human health, but we really just look for anything that's gonna be a toilet disability, that's gonna to have some physical attribute. But basically we want to understand what physical element it is, that's changing in the antigen, that's correlating with the decrease in potency. So it's the virus rupturing, is the bacterial membrane becoming permeable, is the mammalian cell rupturing, what is it that's causing this decrease in potency that we observe throughout processing or unstability. So some of the different ones that we've looked at is basically qPCR, and we look at even a pH shift for some of them has caused that. We're looking for a simple measurement that we can do, you know, in a deal format in association with small-scale optimization to improve the process, and then track the process thereafter.

Interviewer: OK, and so when you're looking for some of these stability things, what kind of knowledge and skills which you feel like is required in order to really find those?

21: I use a lot of spectroscopy, and use basic, I think pretty basic analytical techniques, so like just sometimes you even as simple as a total protein assay of gel, especially when we have a lot of fractionation of different fractions, we're looking at tracking where the antigens going, so sometimes it's even just different centrifugation to separate out different portions of the sample, like a sucrose density base, or just traditional centrifuge, and I also use, and of course a lot of the methods that we use to track the actual titer are ELISA based or plate based, and that's what we try to avoid doing those as much as possible, not only for the time they take, but for the amount of variability that they have.

Interviewer: Sure. Can you think of any non-technical knowledge or skills that you would need?

21: Yeah. I think I was really interested in doing your interview, because this is a question that my graduate advisor asked me when I came back to the university a year or two after graduating, saying you know, what did you not learn that you feel like you were surprised by, and you really need it. And I think a lot of that is more critical thinking, about external influences rather than things you can control in your own lab. So you need to be really aware of the attributes of the sample that are coming in. You might not have control over, but may be affecting your results. So I think being able to work in a more matrix environment, rather than exclusively being able to work on teams that is huge, especially in these larger organizations there's a lot of people involved in the processes, and each person has really useful information. So you really gotta reach out and see what you can learn externally, as well as what you can learn in the lab. And then there's a lot of project planning, so no one wants to help you out if you come to them at the last minute, and say you know, oh I forgot to make the sample like this. You really need to be a good communicator, and plan out in advance how people understand, why it is you're doing what you're doing, get them to buy in on it as well, that you're going to improve their process. And another one is really big here, and was using elements of Six Sigma or like the greenbelts approach. People really want to see that you're really streamlining the work that you need to do, they won't want you mess around doing, you know, 20 experiments when the question they've really been answered with only four or five. And so you really need to be able to be critical about why you're doing each study, and what it's going to tell you. But you also have to put together pieces of puzzle. So have factual tribal knowledge that comes from the operators on the floor, and the R&D people who develop the process initially you have the data boards, where you're getting the data that's collected on the production lots now. And you kind of have to put it all together into a cohesive mechanism or story, to explain what's going on with the process.

Interviewer: Okay, there's a couple of things that I wanna ask about because I am not as familiar, you know a surprisingly in the academic nature with some of the industrial things. You said working matrix environment, can you just tell me briefly what that is?

21: Yes, so you're not necessarily going to be reporting your results to just your advisor, just your boss, right? You're gonna have other people who are vested in it, the results that you indicate may upset someone, so you've got to be really sensitive to how it impacts different areas. You need to think about who you communicate to first, and just make sure that everyone feels like they are respected in their role in the project. So matrix environment just meaning that there's multiple people vested, and with some sense of authority over your work.

Interviewer: Okay, and then the other thing that you mentioned was, I believe you said something like a Greenbelt environment?

21: So it is really into the Six Sigma training. So Greenbelt is like the first step in becoming Six Sigma training after Greenbelt there's a black belt. And it all rolls around the DMAIC methodology, which is define measure analyze improve control, and it really helps you to lay out a project plan, it helps for communication purposes for people to know where the project is, are we still in measure, are we in analyze yet, what are we going to do to control it. So it's basically a common-sense approach, it's very structured, and it avoids letting other people have some scope creep. So if you're doing project and say oh I've been willing to look at this too, ultimately that's not even us to analyze, and if you let that affect your ability to analyze the first question, you're not going to satisfy the people that have asked you to do the work. So using the DMAIC approach kind of helps with that, because you can say, you know the problem we're defining here is this, you know, we may be able to get to that later on, it helps you isolate the work that you're doing.

Interviewer: Okay, you have given a lot of really good information here, and I'm trying to sort of which one I want to go back and ask. You talked about right at the beginning of this conversation, you talked about critical thinking, about external variables, and then kind of talked about you know like where did you get the sample from, and all the things that can impact the experiment, and also working in this kind of matrix team environment. Were those types of things you were referring to with external variables?

21: Yeah, but even more than that, I mean for example, when I was in graduate school, the antigen that I worked with. So I work primarily in vaccines through graduate school. But whatever target protein or target you've worked on, you're not always going to be involved in the complete manufacture of that product. So you're going to need to understand whether it's made at a different site, or in another building at your site, was the process that was used the same one that's always used was something different about this process, where is it controlled temperature, and why and where do we not have temperature control, and why what's the duration of each storage, what are the raw materials that are used, how well characterized are those raw materials, can they marry from manufacturer to manufacturer, does all the elements of a process that can be outside your control, because it's really important to make sure that you don't come up with a false positive So if you identify some attribute that you start to utilize to trend, and then all the sudden it disappears, because it was really just a protein that was in your media that changed. It's gonna be pretty detrimental to your success. So it's really just about knowing all the blind spots, the spots that you don't have hands on.

Interviewer: Do you have general knowledge the skills that are being required for identifying those blind spots? And how to you know obtain the information and decipher that information?

21: I think what we just talked about with the DMAIC methodology, they have tools online that help you organize things, you know it's a main variation, it is a method variation. But I think the other element is just the soft skills that we talked about, I think there's a lot of folks who have a difficult time forming relationships that will help them to get their jobs done. So you know we really have to be cognizant that our communication style affects our work in the end. And we have to tailor our communication based on the environment you might be working in. So if I'm gonna go spend a night on the floor with the guys, the union guys they're working production, it's going to be a lot different conversation, than if I'm working with the regulatory ladies who are submitting and talking to the regulatory authorities. So you just need to be able to kind of discern, you know what's important to those people, how to get their buying, how to have them alert you when something comes up, and just to form that kind of network.

Interviewer: Okay, and then the last thing we want to ask you mentioned project planning, and that was being a good communicator, and then it's called DMAIC method?

21: It's called DMAIC. There's other ones out there like it, that's just the one of them.

Interviewer: OK, so primarily comes down to good communication and this DMAIC method of project planning, is there anything else that you feel like would be included in project planning?

21: I think being flexible is also a good one. I think sometimes we have to give a little bit to get the buying from other people, so if they say, you know, we can support that but right now we're commissioning something new, so our operators are spread then, you move it to next week, a week after, you know, other groups are going to be affected you kind of gotta keep everyone moving forward, but also accommodate where you can.

Interviewer: OK, and then in being a good communicator you've mentioned buying a couple of times, what general skills do you feel like are required to get that buying, and again I know that you've already mentioned things like forming relationships with people, it sounds like discerning who you're talking to, and considering that sort of thing, is there anything else you'd like to add to that?

21: Yeah, I think it would be it always gives the feedback of the work that people have done for you, and what impact it had. So the first time you get someone to support something for you or to help you out with a study, allowing them to see the data that came out of that study, and the conclusions that you made, and what it means for the team going forward, will help them to stay involved and committed to help you in the future. So if they never see any of the work that you've done, then you may not have the same level of the interest in the future studies.

Interviewer: And then you also mentioned that you need to kind of put it all together for a cohesive story, does that feed into the communication, or is that kind of a separate kind of knowledge or skill do you feel like you need?

21: Yeah, I think definitely knowing who you're presenting to is a huge element of bringing it all together. So if you're presenting to the folks that are going to be working the process on the floor, they're going to be concerned with old times, and how long processes, and help them understand why those decisions are made. But if you're talking to someone in finance, you're going to need to understand the cost of goods, and what impact this improvement can have in a dollar fashion. So you just got to really understand and make sure that you're not making improvement in one area to make a huge sacrifice in another area, because ultimately that doesn't benefit the business.

Interviewer: Sure. Can I do a little further into that, you know, what kind of considerations do you need to well consider when you're thinking about that particularly in the financial we're talking to the production people?

21: Well, I think the basic premise that I've come to is using to ask them before you get started on the work. So you know they may have an issue, then we're losing some product here or there, I need to understand where we have flexibility. So can we expand and process this as smaller sub lots? If that's an option, can we use an extra ELISA? Can you schedule smaller batches? Can we you know how can they adjust and then try to work a solution into that, rather than going forward with what you think the best solution might be. Because regardless of whether that is a good solution, if it's not one that the business is prepared to embrace, then it's going to fall on deaf ears.

Interviewer: And then the business there is that referring to any particular individual office or is that just kind of like a market value?

21: It's really referring I think a lot to a certain. If you're working within a site, then it would probably be referring to the site's metrics. So they look at metrics, how many failed batches or how many deviations. So if you're working in a more global environment, there may be different elements of what the business needs to show that they're successful.

Interviewer: In all of those was kind of couched and stemmed of a conversation about how you were talking about mostly stability and development of your parameters that you were looking for. You did also mention troubleshooting was a big component of position, is there anything unique that we haven't really talked about yet that you feel like troubleshooting kind of adding to that in terms of what knowledge and skills you need in order to troubleshoot things?

21: In asking questions, I think being comfortable. I think one of the biggest things for a PhD coming into an environment like an industrial environment, they feel they have to be the expert on everything. And that's definitely not going to get very far, because I think the biggest thing is you have to learn to be comfortable when you don't know anything, and find ways to get that information, and to do it in a way that's conducive to team structure into bringing others along with you. So just being comfortable with what you don't know, asking the right questions.

Interviewer: Okay, so I know we were talking specifically about, I guess your one type of project, is there any other types of projects that you're working on right now that they feel like again would will provide any unique knowledge and skills we haven't talked about yet?

21: I think the only other thing that I thought of as you're talking that hasn't really come up is really related to how industry works compared to academia. And that would just be that, I think it takes a bit, and maybe some people don't really get there to understand that the business will make decisions that don't make science sense. And if you question that, if you appear to critique the business for that and can't get behind it, it will be viewed negatively. Certainly we all want to see decisions made that make comments on science, but a lot of times they're going to tell you, we'll come back, we'll do that in a round 2, or the budget for this project doesn't allow that, or we just need to get to the clinic, or whatever it is. And so you've got to find a way to kind of try to work those things back in later, if you think they're really critical, but do not be seen as someone who can't support the business directives. I think that's a hard thing, lots of people say. I, even myself struggling at first to say "how are we making money here and none of these make sense".

Interviewer: Would it be fair to classify that as more of an attitude that you need to come in with, or that you learn as you work on the job?

21: Oh yeah, I'm sure it's something that has to be seen, but I think if people coming in understand the concept a little bit that it's a business and not an academic lab. It may be if someone told me that going in and then I saw it maybe I would be a little bit more prepared to embrace it.

Interviewer: Okay, and then with the last seven minutes or so here before I let you go, I'd love to just ask you about some of the skills that we've come up with and then if you could just give a very brief, yeah I think that I definitely need that for my job or no that's not as important, and then give a brief kind of explanation. So I know you mentioned communication and team-working skills quite heavily, so how about multitasking skills, do you feel like that's necessary for your job?

21: Yes, definitely. In most cases, even if you're working on a single project, it's gonna have different work streams that you're working on, someone is going to move fast, someone is going to move slow, so you kind of gotta keep tabs, and all of them.

Interviewer: And teaching skills?

21: Yeah, I definitely think that's helpful. I think it's a recognition and it's a different thing to teach someone who is highly technically trained versus someone who is not, so an operator in production versus a scientist 1 or 2. And just kind of catering to what the important information is for each of those types of groups. But then also in that way kind of related to communication. I think one thing that I've heard before about PhDs can do presentations that will use a lot of terminology not only they understand. And so may be kind of teaching in that way, making sure that, for example, if you're presenting to someone three or four levels above you, they should still walk out feeling educated not necessarily confused. So teaching in that way through communication I guess too.

Interviewer: Sure, and how about time management skills?

21: Oh yeah, that's a huge one. It's really easy to get sidetracks about someone else's experiment or maybe even doing favors for other people to try and keep up that, you know environment or supportive network that you've created, so you get to know when you really got to get stuff done.

Interviewer: Sure, and I think you also mentioned analytical, quantitative skills that those were also important.

21: Yes, I think statistics is a weak point that I had coming into the industrial setting. Basic statistics would be really helpful.

Interviewer: Okay, how about writing skills?

21: Yes. I think in graduate school I had no idea how important that would be. I felt very frustrated at the time with my adviser you would spend several rounds giving me, you know scientific critiques, like this word is not a descriptive scientific word, this is a personality trait of a person, this is a you know you need to choose scientific writing terminology, and you need to organize things in a way that explains where you started in your experiment, and what you learned.

Interviewer: Okay, so that was something you thought was valuable too?

21: Yes. I found a couple of people throughout my time so far ask me to read their things repeatedly, because I think they didn't have that opportunity to improve on writing.

Interviewer: An important question I should ask too is when you're communicating your projects ideas, does that happen primarily through an oral channel or through a written channel or both?

21: Both. It depends on who you're talking to. If you're talking to maybe your colleague or your manager, you might do it orally, and be able to kind of dialogue with them, and brainstorm. But there's a lot of prioritization of activities that happens on spreadsheets. So you're going to be able to capture the name, benefit of doing the project, and the risk of not doing project.

Interviewer: Okay, how about general problem-solving skills?

21: Yeah. I mean I think that goes with it to make methodology, making sure that you identify the exact problem, that you're trying to solve, and then making sure that all of your efforts are toward addressing that problem.

Interviewer: Thank you. We're gonna be fair to say that would go with decision-making skills too?

21: Yeah.

Interviewer: And then the final one for you is networking skills, you've talked a lot about networking within your organization, can I ask about networking outside of your organization?

21: Yeah, I think this is the one where I'm working to improve still. I think when I have something I can talk to people about it's pretty easy for me to start up conversations in network, I think it's obviously more difficult when you're just explain the future possibilities. So for example, at conferences, new technologies you might explore, new groups you could maybe work with, and may be a little bit more open-minded about how their solutions or their ideas could fit into your work.

Interviewer: Okay, now that we've had a good warm-up to really just leave mind about things, anything else you can think of as a closing remark about what kind of knowledge and skills you feel like is required for your job/

21: I think the biggest one is just teamwork, you know, I think we're getting a PhD or working pretty isolated I guess, so a lot of times. At least it was my experience you know, you're the one who's really designing experiments, you are not always needing to coordinate with someone else, I think it is very easily become more comfortable doing everything yourself. So that's definitely not compatible with an industrial environment where there's a team for everything. So I think team works a huge one, teamwork and communications.

Interviewer: Okay. Well, thank you very much for your perspectives here, that's the conclusion of the interview. The one thing I will say is that you do want to give you an Amazon gift card and I'll be sending that electronically, is it okay if I sent it to the same email we've been corresponding with? Or do you have another one?

21: That's fine.

Interviewer: And then the last thing that we always ask as well is just since it's very hard to get connected with people in industry, if you have any colleagues, any management or anyone even outside of your organization that you'd feel comfortable sending an email that Kaylee sent to you, I always would ask for you to send that along to other people.

21: Okay.

Interviewer: Thank you very much.

21: How long will it be running through?

Interviewer: Probably at least for another month or two. The qualitative portions, it really just depends on how many people we can get and how quickly. So the worst case scenario is we turn them away for temporarily and then even as early as next year we'll be launching a quantitative survey and we can invite people to take.

21: Okay. And how do you guys see this being rolled out to your university or other universities?

Interviewer: Sure, that's a really good question. Currently the goal of the research is to simply characterize the knowledge and skills that are required for various sectors, so the industry would be where you're invited to. We've been talking to people in academia or gonna be talking to national labs, and as well as some other sectors in track down. The original goal is to disseminate primarily through research publications, but also I have a nice role in the American Chemical Society and so I'd like to get them involved with it too. And specifically at our University I certainly want to see the Auburn University becomes one of the first ones hopefully to really dedicate some explicit training towards an industrial side in a Ph.D program, including potentially some internships with various industries as a part of your PhD experience.

21: Okay, cool. Good luck.

Interviewer: Alright, thank you very much.

**Example 3**

Date: 05092018 KS37

Interviewer: Let's just start with your job title, so what is your official job title?

37: Actually I am between two jobs right now. On Monday, I am starting a new job, which is kind of not as much as chemistry related, but what I'm gonna do is to give you my perspective from my previous job. So my previous job which I finished just this past Friday was the senior scientist at a small company called [company].

Interviewer: Good, and what year did you get your PhD?

37: 2004.

Interviewer: So out of the five traditional research areas, which chemistry division were you in during your PhD program?

37: Organic chemistry.

Interviewer: And what kind of industrial category would you classify your job?

37: Like materials and biotech.

Interviewer: Actually, here are some options for the industrial categories, so things like research and development, analytical services, production, quality control, management, training, marketing, those types of thing.

37: I would say research and development.

Interviewer: Okay, thank you. And generally, how many chemists or scientists do you work with?

37: The team I managed was 4 people, the company as a whole was about 25 people. But not everyone was chemist, so the team that I worked with maybe only 3 are chemists, company as a whole maybe 10 people of chemists.

Interviewer: Okay, sounds good. And could you provide a brief description of your current job? Like what are your responsibilities, and what are your day-to-day activities?

37: Okay, so I have a few different roles. I was a manager of my group, so I was responsible for all the Human Resources related things, like setting goal plans, and doing annual performance reviews and things like that. I was also leading some projects related to development of medical devices, so I was a project manager for a couple of those projects. And additionally, I was responsible for managing the company's intellectual property, so managing patents, filing, things like that. And I also worked as basically kind of consulting with other projects to help them with some of their chemistry needs.

Interviewer: Okay, and thinking about the responsibilities you were talking about, what kind of knowledge and skills do you need to successfully do your job?

37: Well, it's a mixture of things. I mean you need to have the book knowledge, the chemistry or the scientific technical knowledge to do those things. Obviously that's extremely important, you have to have the basic and chemical understanding of the process that you're working on. And you need to, you know, it comes to project management, you have to have project management skills. And that's not something that everyone is able to do well, it's not a skill that everybody has. You have to understand what project management means, how you manage budgets, how to manage time tables, how do you assign people to do different tasks, how do you provide feedback to people, how do you set their objectives from year to year, from month to month, things like that. For the management of the patents and intellectual property, you have to understand that system you have to understand, what a patent is, what a patent isn't, when is the right time to file a patent, what the different types of patents, how do you write a patent, what can go in and what can't go in, so there's a lot of different things you need to do.

Interviewer: Okay, good. So the first thing you had mentioned was book knowledge of chemistry, could you briefly describe some of those knowledge? Not necessarily the specific techniques, but you know what would be included in that?

37: Yeah, because I was working on basically a biomedical materials company, it was a real mix of materials chemistry, polymer chemistry, that we needed to know as well as biology. So if you are looking for specific techniques, I wasn't actually working in the lab, because I was more than a manager in the position. But typically you need to understand polymer, I worked for the polymer chemistry of fluorinated polymers, how to understand the concept of surface roughness of glass transition temperature, characterization polymer blends and compatibility, you need to understand heat compatibility or compatibility of materials, crystallization of materials on top of polymer surfaces, things like that. Reaction of the body to different types of polymers, degradation pathways for different types of polymers in the body, things like that.

Interviewer: Okay, and another big thing that you had mentioned was management skill, both managing group and managing project, so if you have to, how would you define the management skill?

37: It’s a good question, it’s really hard to define it. I would say that you have to know what your goals are, what the goals of your organization or the goals of the project are, and you have to motivate people in your group, people on your team, you have to motivate them to achieve those goals. And sometimes it's not easy to do that, you have to overcome people's natural skepticism, and their natural resistance. And sometimes you have to get people to do things that they don't want to do, you know, they wouldn't ordinarily want to do, you have to learn how to motivate them to do that. So yes, also have to understand people and understand what their motivations are, what their own personal goals are, and try to figure out a way to align that with the work that you are doing. So that's the kind of people management side. And the project management side, it's a bit of a different set of skills, it was really you are responsible for getting a certain amount of work done on particular timetable and under particular budgets. And so that's really about being extraordinarily organized, about being able to understand the flow of work within a project, to be able to get it done from beginning to end, and that's really what the skills are.

Interviewer: Okay, that's really good, and could you break down any more specific skills or knowledge that would be required for the management skill, besides setting goals, motivating people, and being organized?

37: Yes, and you have to be able to provide feedback to people, you have to be able to critically assess the quality of their work, and you have to go through to evaluate someone's suitability for particular task, whether that means interviewing new people for a job, or maybe it means deciding on whether someone should move from one project to another project, you have to have empathy, or you have to be able to put yourself in someone's shoes and see the world through their eyes, which is also sometimes a very hard thing to do. You know on project management, it's kind of a tough one to define, but it's really about you have a goal, and the goal needs to be get executed, and you have to figure out what needs to be done in what order it needs to be done in, and how quickly it needs to be done to enable the project to succeed. So in order to do that, you really have to have a comprehensive view of the entire project, you have to know all the pieces that go into this, what takes time, what doesn't, what's going to be the rate limiting step, and what won't be, what's critically important, and what isn't important, things like that.

Interviewer: Okay, and could you provide an example of how you provide feedback and evaluate others' work?

37: Sure. So the company that I worked at most recently, we had an annual review process that would take place every August. And so what I would do is I would write up basically an assessment of what did the employee do during the previous year, how did it relate to their own goals for the year on their own objectives, how well did they do it, did they make mistakes, did they learn from their mistakes, did they contribute to the group in a positive way or in a negative way. So I would go through that process every year with the people in my group.

Interviewer: Okay, it’s great. And back to the beginning, you had mentioned that consulting was also a part of your job, so what kind of knowledge and skills do you need for this part of the job?

37: That was a kind of informal thing, and that was really about using my expertise, just things that I've learned in graduate school, my postdoc, my previous jobs, using it to provide feedback and provide guidance to people working on other projects with other company. There wasn't really any specific skill involved with those, just my own experience working in different polymer related companies, the materials characterization projects that I've worked on in the past and helping them out.

Interviewer: Okay, and what kind of challenges do you face in some of the day-to-day activities that you had mentioned?

37: Oh, lots of challenges. In the case of project management, it’s not clear all the time what exactly the goal of the project should be. The goal changes from day to day, so that’s one thing. And in terms of managing people, the challenges are that you are working with people in their own personalities and their own things, their own concerns and their own aspirations. And they have requests that sometimes you can't fulfill, and they have wishes that sometimes you can't come to, and sometimes there's conflict between people that you have to help, those are some of the major challenges. So I would say that on the science side, the challenges are kind of much like the challenges that anyone who is the scientist would know, this is just their science, you cannot get a reaction to work, or you got an unexpected product, or something weird happened and you cannot figure out how to do something in the lab, and you worked your way through it, but this is a kind of different thing when you have people related stuff, like what is the goal, what do people think of every project, how are people working, those are the major challenges on this side.

Interviewer: Okay, and is there any specific skills or knowledge that would be required for working with people?

37: Yeah, you have to have really good interpersonal skills, and you have to know kind of how to respond people, and the way to encourage them, not discourage them. You have to know how to communicate really well, communicate extremely clearly.

Interviewer: OK, how would you define the interpersonal skill?

37: You have to know how to be comfortable talking to other people, sometimes very personal subjects, like how are they working, and why they want to do with their careers. You also have to communicate easily with them, and be relaxed with them, you need to discuss something that are uncomfortable or getting them some negative feedback, you have to show confidence and your communications, like you basically show that you are the boss, you know not in a negative way, to do in a positive way. So that's really interpersonal skills, you have to be able to relate to people and see the world through their eyes, give them feedback.

Interviewer: Okay, and could you break down communication skill here like what are the big things that your feel is necessary to the communication?

37: The major thing that's necessary is clarity, you have to be able to convey clearly. They say communication is a two-way street, it's not just about me saying something to you, it's me saying something to you and then making sure that you have heard what I said to you, and understood what I've said to you properly, in the way that I intended it. So that's really what communication is about, it's like I'm stating your concerns really clearly, and making sure that people understands what you said to them, making sure that loop of communication is completed. And a part of that is making sure that people understand that they can come and talk to you, when they need to talk to you about something. They shouldn't feel… when you are a manager, people shouldn't feel nervous about coming to talk to you.

Interviewer: That’s really what we are looking for, and just now you talked about the challenges you face in the day-to-day activities, how do you make yourself prepared to overcome those challenges?

37: Training and practice really. Taking training courses of management skills is helpful.

Interviewer: Did you take any training of management in your workplace?

37: Yeah, my workplace didn't provide me with a kind of management training course that I went to shortly after I started, and my previous workplace before that one provided me with a project management training course.

Interviewer: Okay, could you tell me more about this kind of training course?

37: Yeah, the project management training course I took with my previous employer, that was probably in 2013, was just a three-day course that the employer paid for, and it was basically a project management course designed for scientists and engineers managing technical projects. Because a lot of the times when you take a project management course that's designed for more generic things, like IT projects, or construction projects, or things where there's no technical uncertainty, right? You know it could be done, it's just a matter of what you have to do and when. Science is a bit different, right? There's always as contingencies, so that was of course where we all were sitting in the room and they brought in a project management training guard who came into the course. For the people management training that I did at my most recent employer, they actually sent us away to the training course in another city for four days, and that was a series of seminars, a series of activities that taught about what people's motivations are, and how communication works, how to deduce what someone's motivations, and things like how to communicate clearly.

Interviewer: Okay, and if you have to hire someone to replace you, what kind of knowledge and skills do you think they would need to have?

37: Basically everything that I just reply, they need to have good interpersonal skills, really really good communication skills to be able to state, to convey information very clearly. And they need to be organized, need to understand, they won't understand when they start, they need to be able to quickly understand the project that they are responsible for.

Interviewer: Okay, and when you say to be organized, you mean the skill of time management or other skills?

37: Time management and task management. You have to be able to see kind of into the future what needs to be done at a certain date, and kind of get it started early enough that it's not going to be a problem.

Interviewer: And what specific skill are included in the time management skill?

37: You know it’s hard to put nothing on specific time management skills, just you have to be organized, you have to understand what the flow of a project is, what happens first, what happens next, what happens after that, how long is each thing take, what are the inputs, what depends on, what other things. So it's not really a skill, and other than just being really organized and very meticulous and careful in your planning.

Interviewer: Okay, that's great. And next let's move to the last little section about the interview, we will need another five to ten minutes, is that okay with you?

37: Okay.

Interviewer: So next I'm going to list a couple of skills and I'd like to hear your comments on which you think is important for your job, and any comments you might have about each one of them, is it okay?

37: Sure.

Interviewer: Alright, the first one is multitasking skill.

37: Yes, you definitely to be able to handle different priorities at the same time, different things, different activities going on. I think multitasking is kind of overrated, I don't think there is a clear definition for what the multitasking is.  Some people think multitasking is you do one thing for five minutes, then you do another thing for five minutes, then you do a third thing for five minutes. That's not efficient, it usually leads to mistakes. But the idea of like being able to handle multiple responsibilities, that's definitely important.

Interviewer: Okay, and the next one is presentation skill.

37: Very important.

Interviewer: Why do you think it is very important?

37: You have to be able to communicate your work to other people, and basically convince other people that what you are doing is correct, and then what you are doing is worthwhile. You have to make them understand what the value of what you are doing, basically understand the technical content of what you are doing and understand the value of what you are doing. Presentation skills are very important.

Interviewer: Okay, and in your opinion, how does a good presentation look like?

37: Has to be extraordinarily clear, provide the right level of information, right? Not too detailed, a lot of scientific presentations are too detailed. You have to provide the right level of detail, you have to be extremely clear, you have to emphasize the central message again and again, so that the audience gets it. And it has to be the right length as well, cannot be too long or too short.

Interviewer: Okay, and how about teaching skill?

37: If you are in a management situation, then teaching skills are important, the ability to mentor people is very very important. If you are not in a management position, I don't think they are quite as important. I see men teaching skills and communication skills as being… I'd like teaching skills and presentation skills are basically side by side with one another, they are almost the same.

Interviewer: Okay, a good point. And the next one is analytical and quantitative skill?

37: Important when you work in the technical role.

Interviewer: And how do you think about writing skill?

37: In my most recent job, writing skills were not very important. We produced a very little written material. In many jobs, but I think our company was very unusual for this, everyone just wanted to do everything in PowerPoint or Excel. In many jobs, writing skill is extremely important. I would say overall, it is important.

Interviewer: Okay, thank you. And how about general problem-solving skill?

37: Yeah, very important for anything scientific.

Interviewer: Okay, and how do you feel about decision-making skill?

37: Important to especially for management.

Interviewer: Especially for management?

37: Yeah, someone at lower level, they don’t have much decision-making responsibility.

Interviewer: Got you, and the last one is networking skill.

37: once you in a job, I don’t think it is important. It’s important for getting a job. For my position, it was not important. If you are working in sales or technical services, maybe yes, but my job no.

Interviewer: Alright, great. That's all I have for you today and thank you again very much. We are happy to give you a $10 Amazon gift card for participating in the interview today.

37: That's great, thank you very much.

## Appendix 5: Interview Protocol for Validation Interview

1. According to your responses, you checked the issue box of x item because you have issues with understanding of this one, which is be resilient to criticism and negative feedback. Could you tell me what you are thinking about when you read this item? And why it is not clear to you?

2. What other issues do you have when you read the items of this survey?

For example, is any item too long? Are questions clear or any items need to be reworded?

3. From your perspectives, what questions are not relevant to your profession? What items you think we should remove from the survey?

4. In your opinion, are there any other questions you feel important to your job that we should include in this survey but we haven't?

5. Do you feel that the response options allow you to adequately respond to the questions?

6. According to your responses, you strongly agree with most of the items, if I change the stem from "in order to do my job successfully, it is necessary to…"to "it is important to…", will it affect the extent of your agreement / disagreement?

6. Will you be willing to send out our survey to someone working in industry?

**Appendix 6: Survey Items**

1. build and develop professional relationships inside my organization
2. build and develop professional relationships outside of my organization
3. establish a reputation for myself in my field
4. have an understanding of organizational structures
5. understand ethics as they relate to my projects
6. understand appropriate ethics as they relate to collaboration and publications
7. be aware of and adhere to organization rules and policies
8. evaluate ideas and issues critically
9. find relationships between various sources of information and comprehend subtle meanings therein
10. generate novel ideas
11. acquire new professional skills (e.g. "soft skills") that I currently do not possess
12. develop existing professional skills (e.g. "soft skills") that I currently possess to some extent
13. acquire new technical skills (e.g. new methods) that I currently do not possess;
14. develop existing technical skills (e.g. new methods) that I currently possess to some extent
15. respond to shifting priorities
16. identify problems related to the projects on which I typically work
17. identify solutions to the problems that have been identified related to the projects on which I typically work
18. systematically analyze quantitative data
19. approach new areas and challenges with fearlessness
20. have capacity to deal with competing work demands/challenges

21. be resilient to criticism and negative feedback

22. attempt to solve problems by trying new and transformative approaches

23. set expectations that are realistic

24. be aware of how others are feeling

25. actively listen to others

26. believe in my ability to complete tasks and goals

27. break down concepts and explain them in different ways for diverse groups of people

28. construct curricula to teach/train students/employees

29. establish timeline for a plan in a typical week

30. manage time by consciously prioritizing tasks

31. do my work in an organized fashion

32. categorize information in a systematic and insightful way

33. balance multiple projects at one time

34. be flexible when unexpected challenges occur

35. work with others to accomplish a shared task

36. work with people with different roles and responsibilities in a group to pursue common goals

37. share expertise with colleagues and collaborators

38. motivate/inspire others

39. utilize the influence I have over others to see projects through

40. keep records of the progress of different projects

41. plan out and track the progress of multiple projects

42. identify the challenges and constraints of obtaining financial resources

43. foster group facilitation

44. assess someone's work and provide feedback

45. identify potential sources of funding

47. persuade others within my organization to allocate financial resources

46. conduct "book-keeping" of a budget (i.e. track revenue, expenses)

48. persuade others outside of my organization to allocate financial resources

49. train other employees, interns, or assistants to conduct a certain job

50. set goals within a group for a project or issue

51. effectively search, retrieve, interpret, evaluate, and synthesize scientific literature

52. independently design and carry out projects (reverse)

53. transform technology into business plans/ intellectual property

54. understand chemistry related to my projects fully

55. understand the profession of my work fully

56. analyze and interpret data related to my projects

57. value safety procedures

58. minimize safety risks

59. use precise and clear language when conveying information to someone else

60. organize the content coherently when presenting information

61. communicate topics effectively to different audiences

62. make organized and effective slides for a presentation

63. prepare, edit, and revise written materials

64. present information in a way that makes logical sense

65. convey chemistry to the public

66. am comfortable with the knowledge of the content that I am communicating

67. define a specific goal, action item, purpose, or message that I am trying to convey
68. keep the audience engaged in my presentation
69. know the affect (emotions and feelings) of the audience when presenting information
70. know the background knowledge (related to the communication) of the audience
71. am conscious of how much time I am taking in communicating with/presenting to someone
72. adjust my writing style to fit someone elses' requirements
73. compose an outline of the material prior to writing/presenting it

**Appendix 7: Validation Interview Transcript Example**

2019-10-03 C: Qi Cui

C: According to your responses, you checked the issue box of one item, because you have issues with understanding of this one, which is understand the profession of my work fully. Could you tell me what you think about when you will read this item?

1: So this is really comes from where I'm coming from. So, you know, I'm a professor in chemistry, my job description includes teaching and includes research includes service. Those things are often tension. And so in that sense, if you're looking at this as a skill survey for academia, that will have a different answer than the same question. If you're so looking at it from an industry perspective, and likewise, you are in a national lab, so each of these different organizations have different missions, and that requires somewhat different skill sets. A research university versus a primarily undergraduate institution, for PUI, they've emphasized teaching, typically teaching smaller classes. And you're doing a lot more one -on-one. I teach 360, so that requires a different set of skills. And so that's one piece of it. The other piece of it is oftentimes, what we think of as professional responsibility, we may or may not be aligned with how our institution both evaluates and rewards us. So for instance, my university as a predominant research university, actually promotion from associate to full professor based totally on research productivity and on dollars brought in, you're expected to teach well, but that's a little bit of a variable in terms of, you know, how well you're expected to teach. So as I was saying about the different ways of doing things.

C: So kind of like different type of chemists have different responsibilities for their jobs. So we cannot use a word "profession" to include all these cases, right?

1: So you're still at the development stage of developing. What you really need is understanding how different questions are going to listen. If you're looking at if you've got all the survey data, and you're now trying to do supplemental interviews, figure out why certain questions give very broad all over the answers, that would actually make sense to me. But, you know, my sense if you're not going to be changed yet, then this probably limits to the time spent on trying to figure out how to make it better. So that was a particular thing, I think with that professional in terms of context. If the survey is already gone out broad and you're going to send out a second survey, following up on this, then it's worth a while spending time on figuring out how to improve it. If this is the instrument you're going to get data from, you know, I'm prepared to give you a half an hour, but that might not be the best place to spend time.

C: Yeah. And then I'd like to pick another one: foster group facilitation. What do you think about when you read it?

1: This is a broader question. So certainly, in research, the pushes been towards multidisciplinary research, interdisciplinary research. That requires group skills. And that does require fostering, you know, sort of group participation and so forth. What I see, in engineering departments, they do a lot more of this, because they're preparing them for industry. In chemistry, speaking from my own perspective, the institutions I've worked in, there is no formal development of formal training in group facilitation or group development. I've seen plenty of examples of, say, in the research area, it's unusual for any one person to have all the skill set required to publish. A lot of times you end up having to collaborate with other people to meet goals, because you know, you need a broader skill set. So in that sense, the answer is, yes, I'm acutely aware of that. I'm also aware that within chemistry, and so as I speak from our program, I do not see a lot of signs of this consciously being integrated into the undergraduate curriculum. And likewise, at the graduate level, it's typically left up to the individual professor to integrate it for his group of students.

C: This is really good. And what other issues do you have when you read the items of the survey? For example, is any item too long? Are questions clear or any items need to be reworded?

1: So that the issue here is, there are very few places that I actually have disagree. So what you have with a lot of these statements of expect, especially most of them are written in the positive, is sort of bouncing things up. And again, for example, allocate financial resources. So this is one of those things that in an industrial setting, actually in all settings, resource allocation Is a lot of what the fights are over. Okay, so you have a situation where you do have to work to allocate financial resources, or to get your share of what you need to do a project. This is, frankly, at research university, the biggest single thing, because we rise and fall on our ability to get funding. So what we have for instances is that, you know, I've written strongly agree, persuade others outside my organization to allocate financial resources. This is basically federal funding. But that's not true for a company situation, where will be quite different than looking at internal resources. My organization doesn't have a lot of internal resources. It's relatively small. And so you look at this, is that worth spending a lot of time on? Train other employees, interns or assistants to conduct a certain job. Now, this is part of our educational mission. But from the basis of optimizing one's personal outcomes, this is really only teaching them to do the job that they do for us as research systems. And I've been in tenure promotion meetings, where we do discuss how well students are being trained. But I know darn well that in the case of someone that has three federal grants and doesn't allow his job to train their students, they would get to a promotion. Whereas someone who does a really good job training the students, but doesn't get the funding probably isn't going to get promoted. So this is very specific for an education mission, and does have a context of how long you keep people for. In other words, if you're trading someone who's going to work for you for the future, you have a lot of incentive in long-term, you know, to basically do a good job. Because they can do good work for you. And graduate students, as soon as you know what you're doing, it's time to graduate. And we particularly aware institutions are trying to decrease time to degree, and then wonder why productivity is going down. So these are very context sensitive.

C: I got it. This is a good point. Thank you. And then from your perspectives, what questions are not relevant to your profession? What items do you think we should remove from the survey?

1: Just thinking, if I haven't marked in this question, I would almost certainly have answered with not applicable. Okay, I don't see that I have any that have been removed. So in that sense, if you are aiming for very broad coverage with including industry, and so forth. Because I think, if I remember correctly, your content in the context of what you were able to do is to try and you're looking at student training, and training our students for what they're going to encounter when they get real jobs. So in that sense, I have not mark not applicable, then there aren't any that I've seen. But I'm just talking to say, question 26 establish a reputation for myself in my field, I've got a strongly agree because in academia, our visibility, basically, that's the metric. And in most other things flow from there, within a company situation, I doubt my field is the correct context. Generally, what you're trying to impress is the other people in your company. So there might be field, you know, my fields would do as this chemistry, which if it's chemistry, then it will be applicable. I suspect to soak up well, I would be interested in seeing what that question brings when you have industrial type chemists. My guess would be you might get quite different responses to people and how they read the question.

C: Okay, great. And then in your opinion, are there any other questions you feel important to your job that we should include in this survey?

1: Yeah, so you got evaluate ideas and issues critically. I think that's the only place that I think, you might have used it to relate evaluation. So this is basically on where we are expected to assess subordinates. And truthfully, this is something that professors as a group of very poorly prepared for. And we would benefit by doing some business administration courses or something that basically tackles interpersonal relationships, because this is all about managing people. But there's the other side of the equation, which is that to do your job properly, you also have to basically meet the metrics of people who are evaluating you. So normally in order to do my job successfully, it’s necessary to, we all work either in hierarchies, so very few of us work for ourselves. And that's all different business skill set. We report to the chair, who reports the dean, who voted proposed the provost, reports the president, who reports the Board of Trustees. Generally, you sort of have to make sure that what you're doing aligns with others’ values higher up. Because this is also part of getting resources. It's part of keeping your job if you don't get tenure, and then you are out of a job. And that's probably the most important single thing that sort of impacts us. I think values safety procedures, I've got a somewhat agree. This is one of those things that I think this is actually important. The problem really comes that this particular requirement is not aligned with… there's just a misalignment between institutional support and institutional expectations, where the institution just wants it to be fine, but in a resource limited environment. So that's the other part that. I need to value safety procedures enough that there's no accident that the university is going to then come down on me for, but I'm balancing that against the lack of resources. And the expectation that I'm going to do things, and safety takes time and resources, which institution may not provide. So that you always have these trade-offs, where you balancing various things, to try and get things. So for instance, transform technology, this is I've been through. I've actually started a company with one of my former students that licenses intellectual property. So put them through the university's patent process. Now, I think that's very useful for students to be exposed to. Is it more useful and other things for most chemists, they might depend upon where they're going to be employed. And this might be a big deal. Or if they're employed in software and R&D environment, this can be quite a big deal. If they're employed in a QC, QA lab, but would not need it. Again, [University] is looking at this in terms of making money. And they've decided that no, it's not a money-making proposition, which is probably correct.

C: This is a great one, thank you so much. Do you feel that the response options allow you to adequately respond to the questions?

1: So, if you think about what we spent time doing, there is no, a lot of us if I'd gone through it, I probably would have if there's a box that said, other comments, or whatever, a lot of us would probably haven't been included in those boxes, probably would have taken me about five times as long to do the survey, but that would probably have been much more useful to it.

C: Great suggestion. And do you have any suggestions of how we can improve the response rate and attract more chemists to participate in this study?

1: Yes, this is always the big problem. The problem you have is that you're asking for people's time, which is the most limited resource most of us have. And so now, this actually is going to be a problem for you in terms of assessing the balance of it, because mostly people where you'll get responses that will be either because people want to get out of this system, which I still do it because it's an opportunity to do that. Or because I think it's their civic duty, it's a perfect professional responsibility. And so unfortunately, probably your survey is going to be bias towards those who have the strongest concept of professional responsibility. And it may not adequately reflect respondents who have put those few trying to determine exactly where the field is, in terms of how they view these things. You're unfortunate gonna have a strong self-selected bias. If on the other hand, the goal of this instrument is in guiding curriculum development, then probably actually, people who respond appropriately have spent more time thinking about it. So you may actually get more useful feedback. Whereas someone who is trying to do it a minimum time, either because the bosses told them they have to. And sometimes I don't know how reflective that as you tend to get a snapshot. So I know, your question you asked was get the improving response rate, which was always a problem. Certainly, what you're doing with Amazon gift cards, and so forth. That's probably about the only way you can do this. And as I said, that's a resource issue, I can justify to my wife, who's asking why are you spending time on something like this. So I have three manuscripts for reviews to do, that's going to probably chew up the rest of my day. She's saying why you're doing this and perfectly I regard as professional responsibility. So a survey like this as part falls on that area. But sometimes easier to make the case. And hey, you know, I bought something for you on Amazon, because I did the survey. And I get probably three survey requests a week, lot of it from publishers and from companies doing, a lot of times they're trying to develop sales information for a client. And there are, although they do say that the information is aggregated, not tied to certain people, I sometimes do wonder. So I don't really have a good answer for you on this one. I think what you're doing is about the best that I've seen done. The other thing you might want to do is, if you go to something like an ACS meeting, do a poster, give them a URL and do it by that personal contact. Because it's always easier to say no to something that is relatively anonymous. A lot of people when face-to-face with a person are more likely to give them time. And this is really what you're asking for is people's time.

# Appendix 8: Factor Analysis Output for Pilot Survey Sample

#10 factors   rotate= "oblimin"

Loadings:

| | MR2 | MR3 | MR6 | MR4 | MR7 | MR8 | MR1 | MR5 | MR9 | MR10 |
|---|---|---|---|---|---|---|---|---|---|---|
| [1,] | 0.736 | | | | | | | | | |
| [2,] | 0.663 | | | | | | | | | |
| [3,] | 0.532 | | | | | | | | | |
| [4,] | 0.812 | | | | | | | | | |
| [5,] | 0.673 | | | | | | | | | |
| [6,] | 0.624 | | | | | | | | | |
| [7,] | 0.821 | | | | | | | | | |
| [8,] | | 0.819 | | | | | | | | |
| [9,] | | 0.720 | | | | | | | | |
| [10,] | | 0.617 | | | | | | | | |
| [11,] | | 0.806 | 0.301 | | | | | | | |
| [12,] | | 0.702 | | | | | | | | |
| [13,] | | 0.710 | | | | | | | | |
| [14,] | | | 0.680 | | | | | | | |
| [15,] | | | 0.593 | | | | | | | |
| [16,] | | | 0.655 | | | | | | | |
| [17,] | | | 0.604 | | | | | | | |
| [18,] | | | 0.526 | | | | 0.338 | | | |
| [19,] | | | | 0.757 | | | | | | |
| [20,] | | | | 0.629 | | | | | 0.326 | |
| [21,] | | | | 0.607 | | | | | | |
| [22,] | | | | 0.511 | | | | -0.345 | | |
| [23,] | | | | 0.510 | | | | | | |
| [24,] | | | | 0.506 | | | | | | |
| [25,] | | | | | 0.605 | | | | | |
| [26,] | | | | | 0.774 | | | | | |
| [27,] | | | | | 0.778 | | | | | |
| [28,] | | | | | | 0.744 | | | | |
| [29,] | | | | | | 0.794 | | | | |
| [30,] | | | | | | 0.382 | 0.595 | | | |
| [31,] | | | | | | | 0.509 | | | |
| [32,] | | 0.308 | | | | | 0.676 | | | |
| [33,] | | | | | | | | 0.610 | | |
| [34,] | | | | | | | | 0.620 | | |
| [35,] | | | | | | | | | 0.508 | |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| [36,] | | 0.379 | | | | | | | 0.513 | |
| [37,] | | | | | | | | | 0.717 | |
| [38,] | | | | | | | | | 0.740 | |
| [39,] | | | | | | | | 0.366 | | 0.554 |
| [40,] | | | | | | | | | | 0.633 |
| [41,] | 0.350 | | | | | 0.320 | 0.416 | | | |
| [42,] | | | | | | 0.480 | | | | |
| [43,] | | | 0.369 | | | 0.371 | | | | |
| [44,] | -0.322 | 0.382 | | | | 0.387 | | | | |
| [45,] | | | | 0.328 | | | | | | 0.371 |
| [46,] | | | | 0.313 | | 0.469 | | | | |
| [47,] | | | | 0.445 | | | | | | |
| [48,] | | | | 0.416 | | 0.316 | | | | |
| [49,] | | | | 0.441 | | | | | | |
| [50,] | | | | | | | | | | |
| [51,] | | | 0.375 | | | | | 0.348 | | |
| [52,] | | | 0.470 | | | | 0.347 | | | |
| [53,] | -0.346 | | | | | | | 0.357 | | |
| [54,] | | | | 0.351 | | | | 0.363 | | |
| [55,] | | | 0.310 | | 0.313 | | | | | |
| [56,] | | | 0.338 | | | | | 0.437 | | |
| [57,] | 0.325 | | | | | | | | | |
| [58,] | | 0.448 | | | | | | | | 0.442 |
| [59,] | 0.358 | | 0.306 | | | | | | 0.404 | |
| [60,] | | 0.302 | | | -0.375 | | | 0.376 | | -0.301 |
| [61,] | | | | | | | 0.307 | | 0.308 | |
| [62,] | | | | | | | | | | |
| [63,] | | | | | -0.431 | 0.333 | | 0.348 | | |
| [64,] | | | -0.337 | | | | | | | |
| [65,] | | | | | 0.358 | | | | 0.418 | |
| [66,] | | | 0.363 | | | | | | | 0.316 |
| [67,] | | | | | 0.335 | | | | | |
| [68,] | | | 0.456 | | 0.350 | | | | | |
| [69,] | 0.401 | | | | | | 0.430 | | | |
| [70,] | | | | | | | 0.425 | | | |
| [71,] | | | | | 0.336 | | 0.449 | | | |
| [72,] | | | 0.354 | | | | 0.341 | | | |
| [73,] | | | | 0.450 | | | 0.348 | | | |

**Appendix 9: Factor Structure in Pilot Study**

Factor 1: Community Impact

Q1, Q2, Q3, Q4, Q5, Q6, Q7, Q53, Q57

1. build and develop professional relationships inside my organization

2. build and develop professional relationships outside of my organization

3. establish a reputation for myself in my field

4. have an understanding of organizational structures

5. understand ethics as they relate to my projects

6. understand appropriate ethics as they relate to collaboration and publications

7. be aware of and adhere to organization rules and policies

53. transform technology into business plans/ intellectual property

56. value safety procedures

Factor 2: Critique Ability / Honing of Skills

Q8, Q9, Q10, Q11, Q12, Q13, Q44

8. evaluate ideas and issues critically

9. find relationships between various sources of information and comprehend subtle meanings therein

10. generate novel ideas

11. acquire new professional skills (e.g. "soft skills") that I currently do not possess

12. develop existing professional skills (e.g. "soft skills") that I currently possess to some extent

13. acquire new technical skills (e.g. new methods) that I currently do not possess;

44. assess someone's work and provide feedback

Factor 3: Problem Solving

Q14, Q15, Q16, Q17, Q18, Q51, Q52, Q64, Q66

14. develop existing technical skills (e.g. new methods) that I currently possess to some extent

15. respond to shifting priorities

16. identify problems related to the projects on which I typically work

17. identify solutions to the problems that have been identified related to the projects on which I typically work

18. systematically analyze quantitative data

51. effectively search, retrieve, interpret, evaluate, and synthesize scientific literature

52. independently design and carry out projects

63. present information in a way that makes logical sense

65. am comfortable with the knowledge of the content that I am communicating

Factor 4: Achievement through Resiliency

Q19, Q20, Q21, Q22, Q23, Q24, Q47, Q48, Q49

19. approach new areas and challenges with fearlessness

20. have capacity to deal with competing work demands/challenges

21. be resilient to criticism and negative feedback

22. attempt to solve problems by trying new and transformative approaches

23. set expectations that are realistic

24. be aware of how others are feeling

47. persuade others within my organization to allocate financial resources

48. persuade others outside of my organization to allocate financial resources

49. train other employees, interns, or assistants to conduct a certain job

Factor 5: Conveying a Point

Q25, Q26, Q27, Q67, Q68, Q72

25. actively listen to others

26. believe in my ability to complete tasks and goals

27. break down concepts and explain them in different ways for diverse groups of people

66. define a specific goal, action item, purpose, or message that I am trying to convey

67. keep the audience engaged in my presentation

71. adjust my writing style to fit someone elses' requirements

Factor 6: Planning skill

Q28, Q29, Q42, Q43, Q46

28. construct curricula to teach/train students/employees

29. establish timeline for a plan in a typical week

42. identify the challenges and constraints of obtaining financial resources

43. foster group facilitation

46. conduct "book-keeping" of a budget (i.e. track revenue, expenses)

Factor 7: Organization / Impactful Presentation

Q30, Q31, Q32, Q41, Q69, Q70, Q71, Q73

30. manage time by consciously prioritizing tasks

31. do my work in an organized fashion

32. categorize information in a systematic and insightful way

41. plan out and track the progress of multiple projects

68. know the affect (emotions and feelings) of the audience when presenting information

69. know the background knowledge (related to the communication) of the audience

70. am conscious of how much time I am taking in communicating with/presenting to someone

72. compose an outline of the material prior to writing/presenting it

Factor 8: Working and Communicating as a Team

Q35, Q36, Q37, Q38, Q59, Q61, Q65

35. work with others to accomplish a shared task

36. work with people with different roles and responsibilities in a group to pursue common goals

37. share expertise with colleagues and collaborators

38. motivate/inspire others

58. use precise and clear language when conveying information to someone else

60. communicate topics effectively to different audiences

64. convey chemistry to the public

Factor 9: Miscellaneous Factor

Q33, Q34, Q39, Q40, Q45, Q54, Q56, Q58, Q60, Q63

33. balance multiple projects at one time

34. be flexible when unexpected challenges occur

39. utilize the influence I have over others to see projects through

40. keep records of the progress of different projects

45. identify potential sources of funding

54. understand chemistry related to my projects fully

55. analyze and interpret data related to my projects

57. minimize safety risks

59. organize the content coherently when presenting information

62. prepare, edit, and revise written materials

**Appendix 10: Factor Structure for Quantitative Study**

Efa7

(1) 2, 3, 6, 10, 42, 45, 46, 47, 48, 49

(2) 58, 59, 60, 61, 62, 63, 65, 67, 69

(3) 1, 4, 7, 11, 12, 23, 29, 30, 31, 64, 66, 68, 70, 72

(4) 13, 14, 16, 17, 18, 51, 52, 54, 55

(5) 15, 20, 33, 34, 35, 36, 37, 39, 40, 41

(6) 21, 24, 26, 28, 38, 43, 44

(7) 5, 56, 57

(0) 8, 9, 19, 22, 25, 27, 32, 50, 53, 71

Factor 1. Responsible Conduct of Research (RCR) and Ethics PA2

X2: build and develop professional relationships outside of my organization

X3: establish reputation in my field

X6: understand appropriate ethics as they relate to collaboration and publications

X10: generate novel ideas

X42: identify the challenges and constraints of obtaining financial resources

X45: identify potential sources of funding

X46: conduct "book-keeping" of a budget (i.e. track revenue, expenses)

X47: persuade others within my organization to allocate financial resources

X48: persuade others outside of my organization to allocate financial resources

X49: train other employees, interns, or assistants to conduct a certain job

Factor 2. Communication skills     PA4

X58: use precise and clear language when conveying information to someone else

X59: organize the content coherently when presenting information

X60: communicate topics effectively to different audiences

X61: make organized and effective slides for a presentation

X62: prepare, edit, and revise written materials

X63: present information in a way that makes logical sense

X65: am comfortable with the knowledge of the content that I am communicating

X67: keep the audience engaged in your presentation

X69: know the background knowledge (related to the communication) of the audience

Factor3. Management skills (self-management)     PA7

X1: build and develop professional relationships inside my organization

X4: have an understanding of organizational structures

X7: be aware of and adhere to organization rules and policies

X11: acquire new professional skills (e.g."soft skills") that I currently do not possess

X12: develop existing professional skills (e.g."soft skills") that I currently possess to some extent

X23: set expectations that are realistic

X29: establish timeline for a plan in a typical week

X30: manage time by consciously prioritizing tasks

X31: do my work in an organized fashion

X64: convey chemistry to the public

X66: define a specific goal, action item, purpose, or message that I am trying to convey

X68: know the affect (emotions and feelings) of the audience

X70: be conscious of how much time I am taking in communicating with/presenting to someone

X72: compose an outline of the material prior to writing/presenting it

Factor4. Research ability/technical knowledge and skills PA3

X13: acquire new technical skills (e.g. new methods) that I currently do not possess;

X14: develop existing technical skills (e.g. new methods) that I currently possess to some extent

X16: identify problems related to the projects on which I typically work

X17: identify solutions to the problems that have been identified related to the projects on which I typically work

X18: systematically analyze quantitative data

X51: effectively search, retrieve, interpret, evaluate, and synthesize scientific literature

X52: independently design and carry out projects

X54: understand chemistry related to my projects fully

X55: analyze and interpret data related to my projects

Factor5. Survival skills PA6

X15: respond to shifting priorities

X20: have capacity to deal with competing work demands/challenges

X33: balance multiple projects at one time

X34: be flexible when unexpected challenges occur

X35: work with others to accomplish a shared task

X36: work with people with different roles and responsibilities in a group to pursue common goals

X37: share expertise with colleagues and collaborators

X39: utilize the influence I have over others to see projects through

X40: keep records of the progress of different projects

X41: plan out and track the progress of multiple projects

Factor6. Interpersonal skills / team science skills PA1

X21: be resilient to criticism and negative feedback

X24: be aware of how others are feeling

X26: believe in my ability to complete tasks and goals

X28: construct curricula to teach/train students/employees

X38: motivate/inspire others

X43: foster group facilitation

X44: assess someone's work and provide feedback

Factor7. Valuing safety PA5

X5: understand ethics as they relate to my projects

X56: value safety procedures

X57: minimize safety risks

Factor8. (other: low loading items)

X8: evaluate ideas and issues critically

X9: find relationships between various sources of information and comprehend subtle meanings therein

X19: approach new areas and challenges with fearlessness

X22: attempt to solve problems by trying new and transformative approaches

X25: actively listen to others

X27: break down concepts and explain them in different ways for diverse groups of people

X32: categorize information in a systematic and insightful way

X50: set goals within a group for a project or issue

X53: transform technology into business plans/ intellectual property

X71: adjust my writing style to fit someone elses' requirements

# CHAPTER 5: THE DAILY EXPERIENCES OF NEW DOCTORAL HIRES TO UNDERSTAND TRANSFERABLE ON-JOB SKILLS IN CHEMISTRY-RELATED CAREERS

## Introduction

Doctoral chemistry graduate students have many diverse career paths that they can take after graduation. Even though academic research is commonly viewed as the preferred career path for doctoral students, more than half of them enter careers in industry, government, or other job sectors without searching for a postdoctoral position. The national distribution of chemists based on data from the NSF's Survey of Doctorate Recipients shows that the majority of graduates end up with industrial positions immediately following their chemistry doctoral education.[1] Many doctoral chemistry students fail to take opportunities in non-academic careers because they receive career guidance from their advisors, which is concentrated on academia. The scanty understanding of career options exacerbates labor market imbalances by encouraging students to blindly pursue faculty careers[2-3]. In order to prepare students for diverse professions, chemistry educators need to recognize more career possibilities so they could provide more information to students regarding multiple career options.

For those seeking information on career options, it is well worth consulting the U.S. Department of Labor's Occupational Outlook Handbook.[4] The handbook offers a good summary of job descriptions, educational requirements, salaries, and benefits of jobs. However, the job options are limited and most of the information is described briefly. The UK's biggest graduate career website, PROSPECTS[5], provides detailed information about job options with responsibilities, salaries, qualifications, skills, previous work experience requirements, and career prospects. However, all job postings are grouped in one category without distinguishing between *undergraduate* and *graduate* degree requirements. Another American Chemical Society (ACS) website[6] provides more details about chemists' daily activities for different types of chemistry careers, but the mix of chemists with a wide range of work years makes it less useful for new chemistry doctoral graduates. ACS[7] also maintains a website which includes a plethora of career options for *doctoral* students. This website supplies information regarding job responsibilities, duties and professional skills, but there is a limited connection to everyday experiences and scientific practices for chemists. Thus, a study examining the daily tasks, activities, and potential careers in chemical sciences for new doctoral hires is needed.

In addition to identifying and understanding possible career paths in chemical sciences, it is necessary to recognize what skills are expected to succeed in these jobs. There exists a number of research studies[8-10] dedicated to studying the on-job skills that doctoral students need. These studies are essential for obtaining an overall view of the skills required upon graduation, but instead of focusing exclusively on chemistry, they spread across multiple disciplines. Though researchers have identified some valuable on-job skills, they rarely report the definition of those skills in depth. Most of these studies offer general skill lists developed by experts[11] without explanation of specific skills. Similarly, the list of skills is based on the data collected from broad surveys of graduate students[12,13], yielding limited value to the targeted population. While broad STEM studies are valuable, it is important to conduct discipline-specific research of identifying on-job skills.

Research into the factors that influence students' success in jobs is abundant.[14,15] However, these studies are generally not specific to doctoral students. While some overlap in requisite on-job skills between doctoral chemists and other students is expected, jobs that require a Ph.D. versus other degrees are looking for a different set of skills. This raises the question of how to apply the findings of studies that mostly focus on non-doctoral students to doctoral students. Thus, it is essential to explore and get an insight into the doctoral chemists' daily activities and the requirements for completing their specific tasks.

Knowledge of the required on-job skills and day-to-day activities will help newly graduated doctoral students locate the most suitable jobs and improve the chances of their success in an ever-increasing competitive job market. Most studies tend to report only on employers' expectations for hires across multiple disciplines.[16,17] Human resource managers and employers are fully aware of the skills needed for a specific job. However, the employees are the ones who not only know the job skills but are more aware of the day-to-day activities and requirements of a particular job. The exploration of daily workplace practices of new hires (worked less than two years after graduation) would provide more direct and practical guidance for fresh doctoral graduates. Furthermore, there is an obvious difference of required skill sets between experienced employees and new hires. Therefore, the current study focuses more on the new hires' perspectives regarding job skills in light of their day-to-day activities.

Based on these considerations, we pose the following research questions:

(1) What are the daily experiences of new doctoral hires in typical chemistry-related careers?

(2) What transferable on-job skills do new chemistry doctoral hires perceive to be important on their jobs?

### Theoretical framework

The goals of this study align with the theory of socialization. In 1957, Merton, Reader, and Kendall[18] defined socialization as "the processes through which [a person] develops [a sense of] professional self, with its characteristic values, attitudes, knowledge, and skills which govern [his or her] behavior in a wide variety of professional (and extraprofessional) situations". In 1976, Bragg[19] explained that "the socialization process is the learning process through which the individual acquires the knowledge and skills, the values and attitudes, and the habits and modes of thought of the society to which he belongs".

Socialization occurs in job sectors through formal and informal experiences as doctoral hires to learn knowledge and skills required for their work, interact with colleagues, and integrate knowledge and skills into the activities of their own jobs. Similarly, graduate school also has responsibilities to help doctoral students understand the nature of different careers as an explicit part of the socialization experience for their graduate education. In this study, the theory of socialization could inform the on-job ways that provide new doctoral hires with more systematic preparation, more focused trainings, and more explicit feedbacks for their chemistry careers.

## Methods

### Participants and settings

To help newly graduated doctoral chemistry students understand the possible career paths and transferable on-job skills in different chemistry-related careers, it is important to purposefully sample new doctoral hires from academia, government, and industry. The participants of the study were new hires with a doctorate in chemistry and had worked for less than two years in various job sectors right after graduation. A total of six doctoral chemists (three males and three females) participated in this study (Table 15). The sample came from a variety of chemistry areas: biochemistry, analytical, physical, inorganic, and organic chemistry.

**Table 5. Background information of Participants**

| Participant* | Gender | Chemistry area | Job sector | Job title |
|---|---|---|---|---|
| Bella | Female | Inorganic chemistry | Academia | Assistant professor |
| David | Male | Biochemistry | Government | Forensic scientist |
| Eric | Male | Computational chemistry | Industry | Entry level scientist |
| James | Male | Analytical chemistry | Industry | Entry level scientist |
| Nancy | Female | Organic chemistry | Government | Physical scientist |
| Olivia | Female | Organic chemistry | Academia | Lecturer |

*Pseudonym was used to maintain anonymity of participants.

**Data collection**

Chemists were invited via email to participate in 30-minute semi-structured interviews[20] conducted electronically and recorded with the permission of participants according to IRB regulations (#17-362, Auburn University). The research was conducted ethically with the informed consent of the participants. Pseudonyms were used to maintain the anonymity of the participants. The semi-structured interview approach was used to explore individual experiences and perceptions which provided extensive details.[20]

**Data analysis**

All interviews were recorded and transcribed verbatim. Thematic analysis[20] of the six transcripts were undertaken using the qualitative data analysis software Dedoose through a multistage coding process. Thematic analysis can be used to identify the key transferable on-job skills that participants perceive to be important in their jobs.[18] The first step of coding involved reviewing the interview transcripts thoroughly and highlighting salient features of the data, which were related to the research questions. Then the data was provided with codes. Next, a list of codes was compared and sorted into categories. Finally, through the process of synthesizing similar categories, themes were derived depending on how they related to the research questions.

## Results

### Interview summary

These interviews covered various job sectors, positions, as well as research areas of participants in the U.S. chemistry-related workplace. Interview summaries listed below provide the daily experiences of new doctoral hires in chemistry careers. These interviews serve as a valuable tool for fresh graduates in understanding different possible careers in chemical sciences as well as the socialization experiences in different jobs.

1. David: forensic scientist in a state agency

David works at one of the facilities of a state agency, which employs about 200 scientists across the state. He is a forensic scientist and the head researcher of the firearms department. For half of his responsibilities, David is in charge of case work which involves homicides, violent assaults or violent crimes as a forensic scientist at the agency. He performs scientific analysis of the suspected firearms to determine if a bullet or cartridge case was used in a crime. The other half of David's responsibilities is to develop new methods of forensic firearm analyses as the head researcher in the firearms department. He has several on-going projects; spectroscopy plays an important role in these projects to make forensic science more objective, as opposed to the current method relying more on people's opinions. His job is to cultivate new scientific approaches to incorporate instruments, such as Inductively coupled plasma mass spectrometry (ICP-MS) into firearms analysis.

Based on standard operating procedure, the agency offers a 1-2-year training program for every new employee regardless of their educational background. The purpose is to help new hires acquire skills from forensic work. This standard training provides new hires hands-on, work-based mock scenarios. New hires try to solve these cases and take a variety of practical examinations to finish the training program.

David encounters two main challenges in his daily tasks. Though he was trained to write scientific papers in graduate school, he is now challenged with writing technical reports to non-scientists, such as defense attorneys, defendants, juries, and judges. However, the on-job training program offers a report-writing module that teaches new hires writing skills addressed to a diverse audience. The other challenge he faces is to be aware of how much money is spent on research. The typical instruments for firearm analysis are direct analysis in real time (DART) and ICP, which are costly. It is difficult for an underfunded forensic agency to adopt them. Therefore, David must come up with new methods within the budget that forensic labs could inexpensively adopt and write grant proposals for the National Institute of Justice to obtain more funding.

2. Bella

Bella is an assistant professor of instruction at a 4-year comprehensive university. She teaches general chemistry courses and manages laboratories for general chemistry. To plan a course, she prepares lecture materials to line up with labs; modifies slides and assignments that are appropriate for students; and prioritizes certain topics that students struggle with in her class. As a general chemistry lab manager, Bella develops learning objectives for students as well as teaching assistants to ensure they understand the expectations for a given experiment. She also manages

TAs to make sure they can interact effectively with students. Additionally, lab safety is an important aspect that she focuses on in her lab.

The biggest challenge for Bella is to finish multiple daily tasks within constrained time frames. Because she enjoys her job, she stays in her office longer than her designated office hours and ends up working late. In order to keep herself on track and accomplish everything, she made a to-do list to get these tasks done in whatever order. Another challenging as well as fun part for her job is to develop new things for labs. She takes time to re-evaluate the learning goals of certain experiments, make extra materials for students, and change the existing labs gradient.

3. Eric

Eric is an entry level scientist in a Contract Research Organization (CRO) specializing in bioanalytical services. His daily tasks include analyzing various biomaterials, biometrics, and pharmaceutical compounds. On a day-to-day basis, he takes samples from the clients, prepares assays, and analyzes the concentration of compound in the matrix. To complete these tasks successfully, he uses chromatography frequently, High Performance Liquid Chromatography (HPLC) in particular.

Since his background is in computational chemistry, which is not related to his current job, he was trained in his company to operate the instruments for analysis and automation systems for assay preparation. At the same time, he learns new computational chemistry knowledge on the job. It helps Eric to prepare for his next position that matches his research in graduate school.

The most challenging thing he faces is the comparison of theoretical calculations with the experimental results. His responsibility is to design the most stable molecular structure and compare it with experimental research. However, there are many times the process fails when he compares the designed structure to the real-world crystal structure. As a result, he needs to re-design and re-calculate everything from the beginning. Literature searching and review facilitates him become more prepared to overcome the challenges. Reliable literature could help him find the potential factors that are relevant to the subject being explored.

4. Nancy

Nancy works as a mechanical scientist for the U.S. environmental protection agency. She is responsible for monitoring radiation levels of different grasses and waters across the United States. When she has samples to analyze, she estimates how long the process may take and schedules a lab time; works it through the standard operating procedure of diffusion method; takes the sample to the counting room. Furthermore, Nancy is also a member of a reference lab committee where she is responsible for establishing certain standard operating procedures and figuring out what path they want to take.

When she first started, Nancy received training from every lab and learned about the operations of the instruments. The training program checks if new hires could pass the analysis until they become certified on different methods. Nancy is also training to be a standard chemist for quality assurance in her current workplace. In addition, she is required to get 80 hours on continuing education.

The challenge that Nancy faces is to start over the experiment if she skips one step of the fusion method or the quality assurance analysis is unsuccessful. To overcome the challenges, it is necessary for her to pay attention to everything about the experiments, follow the standard procedure, have everything prepared, and take safety seriously to avoid the domino effect.

5. James

James is an entry level scientist in a company specializing in drug metabolism and pharmacokinetics. On a daily basis, he develops methods and analyzes samples to support pharmacokinetics study for drug discovery. In order to develop new drugs for humans, he performs animal studies with the new drugs first. To understand how a drug can be metabolized, he optimizes the drug sample preparation method. He collects sample data at different time points during several days and then uses instruments to determine the concentration of the drug samples in the plasma.

His company provides hands-on training of various instruments that the senior scientists teach new hires step-by-step. In terms of HPLC, he learns the techniques of determining the most suitable particle size and the mobile phase inside a column, as well as dealing with carryover issues.

The challenges that he comes across in his job are the carryover issue and the crosstalk issue when he develops a drug sample preparation method. The carryover issue is caused by either the autosampler system or the insoluble compound in the column. The crosstalk issue raises when the mass spectrometer cannot differentiate similar compounds. James thinks that teamwork is essential to overcome the challenges because the short turnaround time in industry does not allow employees to spend too much time on one task. Thus, James asks for help from his supervisor in order to get his work accomplished sooner.

6. Olivia

Olivia is working as the lecturer in a public research university. She is teaching three undergraduate level courses, including one organic biochemistry course for non-chemistry major students. Her day-to-day activities include lecture preparation, emails responses, and coordinating meetings with other faculty and instructors. In her daily routine, she answers student questions about the course content and how to be successful in the course. To prepare lectures, Olivia builds slides based on the publisher's material with the goal of making them visually appealing and mentally appropriate to keep students' attention. Additionally, she advises students to achieve their career goals or adjust their career plans.

Olivia had some unique training as a graduate student. She enrolled in the preparing future faculty program and did a mentorship with a local instructor to see how he ran and set up his class. She also took a variety of teaching courses, which included academic job searching and developing a college syllabus. Moreover, she sought out higher-level TA responsibilities and taught a class as the primary instructor during the summer semester. In addition, she and other graduate students developed a club to study articles in chemistry education related journals. The articles on chemistry teaching and pedagogy helped them to improve their own teaching strategies. Eventually, they built an online course that is being taught at their university.

The big challenge that Olivia has are the time constraints for each lecture because it is difficult to go through all the slides within the limited class time frame. Additionally, she struggles to figure out the best order to present the concepts. Olivia prepares each chapter before starting the class and manages her time very well. She has a copy of each course calendar and plans ahead of time to ensure everything can be done a couple of days before the class.

**Transferable on-job skills required by new doctoral hires**

From the interview summary of these six new doctoral hires, four themes arose that explained the on-job skills influencing success in the common chemistry-related workplace. (see Figure 1). These themes describe how they play a key role in the participants' daily tasks.

1. communication skills

Communication skills consist of oral and written forms. One important thing that should be paid attention to is being aware of the audience of both forms. For our participants, Olivia teaches non-chemistry major students who came in with different levels of chemistry knowledge. It is helpful for her to be able to explain chemistry content knowledge to students with different backgrounds. Similarly, Bella finds it important to understand the students' or TAs' experiences and purpose so that she can integrate the information into conversations.

*Whether I'm talking to students or whether I'm talking to TAs is being able to understand where the other person is coming from, and what information they need most urgently, and then integrating that into everything that I need to say to them ~Bella*

In terms of government scientists, David writes technical reports to explain the experiment results to non-scientists such as defense attorneys, prosecutors, juries, defendants, and judges. Though he needs to write reports in a scientific way, the reports also need to be understandable by the people in other fields. Nancy believes that it is important to communicate with lab technicians in and outside of her research group and with academic people when she goes to a conference or submits a scientific paper.

*You put it into a step-by-step direction, so a non-trained person would be able to come do it, those are the skills I'm talking about. We can write it for people at the Journal of Organic Chemistry, but you write it for maybe a lab technician, it's in between technical and non-technical skill. ~Nancy*

Other than being aware of audience, conveying ideas clearly was mentioned by Bella when she talked about oral communication. Participants discussed different aspects of writing skills depending on the written materials that they work on at their jobs. Bella prepares experiment notes for TAs. She tends to make them brief, clear, and the topics prioritized. David writes technical reports to diverse audiences and is trained to write standardized reports to non-scientists.

*Everything's very standardized, so that's what we do here, very standardized. It's definitely not like academia, lots of freedom.* *~David*

2. organizational skills

Participants mentioned time management frequently when they talked about organizational skills. Olivia organizes class flow. She puts together organized lectures that fit an appropriate timeline. At the same time, she makes all the components of her class organized, such as the syllabus and the university policies.

*Having a course calendar arranged, developing a syllabus that outlines all the information they need to know, making those kinds of decisions, what kind of policy am I going to incorporate into my class, how am I going to respond to various scenarios like missed class, missed tests, late assignments, etc.* *~Olivia*

In order to complete these in a timely fashion, Olivia plans ahead of time. She has course calendars and a weekly schedule to start working a couple of days in advance. She also schedules most of her appointments around the same time frame.

Before managing her time, Bella will make sure that she knows the learning objectives with a certain experiment. She makes her own focus list to accomplish these tasks, but she is flexible with the amount of tasks that she could complete and the order of which is the most important.

*So in order to keep myself on track and accomplish everything I want to accomplish during this week and spring break, I made myself a list of, I call it like a focus list, and it's kind of just a to-do list, but it allows me to work in whatever order I need to, as long as I'm working on one of these tasks, I'm accomplishing something. So I do have like running lists of things that need to get done, and I just sort of allow them to take the time that they need, because I don't necessarily know how long something's going to take, especially if I decide, oh this lab is not good, I need to totally redo the thing, and once I start looking into it, it's harder or easier than I expected, you know, time can sort of change on me.* ~*Bella*

In government, the deadlines are not as strict as in academia. Nancy is self-motivated because she does not want to procrastinate. One of the biggest things she realized is prioritizing the things that she needs to accomplish. Furthermore, she works on everything quickly to get it done.

*Actually I'm gonna grasp on everything you need to get done, like this meeting that we had, we have an audit coming up, and I was in the middle of getting prepared for that, and I let this completely slipped my mind. So they have all types of different ways to use your calendar on your Microsoft Outlook, your cell phone, whatever you have to do to make sure that you don't forget anything that you are supposed to do.* ~*Nancy*

3. Problem-solving skills

To solve problems for a specific issue in a project, Eric prefers to search and review literature and figures out solutions himself. When he faces some trouble, he searches reliable literature related to his field because it will give him the most important factor to get a final solution. Contrary to Eric, James is willing to ask for help from his supervisor. From his perspective, industry has a very short turnaround time, which is quite different from academia. Industrial chemists collaborate closely in order to get work done sooner.

*I don't know how to do it, so I will talk it to my supervisor, he will give me some suggestions because he has been working in this area more than twenty years, he knows all kind of compounds and knows why those compounds have weak signals ~James*

In a state agency, David faces funding problems in his workplace. It is difficult for an underfunded state agency to adopt expensive instruments for their analysis. In order to achieve the desired results of the research project, it is important for David to be creative. He must come up with ideas of using what he has within the budget to solve problems. Additionally, he writes grant proposals for the National Institute of Justice to obtain more funding.

*Because like I was saying the labs are underfunded, we don't have a lot of money to spend, because we are state agency. So a lot of times you've got to come up with your own ideas, if something happens or if you need something, you are not always going to have what you need, like the instrument that you need or the piece of equipment that you need. So a lot of times you have to come up with an idea be resourceful, and come up with some kind of idea that uses what you have to solve your problem. So there's a lot of problem-solving skills that's required, I would definitely do that. ~David*

4. teaching/training skills

Depending on whom to teach/train, participants talked about different subskills. To prepare a course for undergraduate students, Olivia first needs to know the realistic expectations of her students' knowledge, how much time students can devote to the class, and what they expect from her. Next, she starts with the publisher's PowerPoint slides and re-develops them based on the slides from last year. She keeps working on the slides to make them visually appealing and mentally appropriate for students. Furthermore, she incorporates several instructional strategies into her class to help students be successful.

*I design a lot of in-class questions, so I have to build questions for every day as well as incorporate homework assignments, so I have to be able to manage the online homework system, assigning the homework through the online homework system, integrating it into our learning management system. We use Blackboard, so I need to be Blackboard competent, writing and grading exams.* ~*Olivia*

In addition to course preparation, advising students is another important aspect of teaching for Olivia. In order to give proper advice, she needs to know the requirements for different majors in the university. These include the courses that students need for their major and the timeline to fulfill all the requirements.

*So understanding how the university requirements work and how the registration process works. I need to figure out how to advise them about when to register, how to register, what to register for, when classes are offered, when they are not offered.* ~*Olivia*

Moreover, Olivia is responsive to emails and in-person questions. Interpersonal skills are another essential component when teaching students in an academic institution. Olivia is trying to be personable so that students are not too intimidated to talk to her.

Teaching for Bella is more about preparing the laboratory for undergraduate students and training TAs to be effective teachers. She develops learning objectives to make the goals very clear for TAs. She determines what is important, translates it into learning objectives, and makes those learning objectives align with the experiments. After developing the learning goals, she also prepares a crash course in lab calculations to train TAs.

*So I sat down with the TAs and I said, you know, these are the objectives of what is going to happen this week, and here's what you need to know, many of them expressed that they didn't remember electrochemistry, they had done it a long time ago. So I ended up giving them kind of a crash course in how to do the calculations that were relevant to the lab, so that they would be able to help the students.* ~*Bella*

There are a variety of topics that are important for students to learn in general chemistry. However, the time constraint makes it difficult to cover all of these topics. Thus, being able to prioritize topics is an important skill for Bella to have to prepare the course contents. Most of the time, she tends to focus on topics that students struggle with in class.

*I need to know how to prioritize certain topics. Oftentimes they touch on a bunch of things in general chemistry, but which are the ones that are the most important, which are the ones those students are going to use later, and then also what's important in terms of what students struggle with. So I don't want to spend a lot of time on geometry, even though they're going to need it later, they don't really struggle with that. So I'll try to focus on things and give them more practice with things that they have trouble with, rather than focusing on something they might see as easy.* ~*Bella*

The teaching skills involved in David's job are to train police officers. The local police departments and sheriff's offices submit the collected evidence to the state agency of forensics; however, they are not trained very well on how to complete it. Therefore, David and his colleagues go out and train them about it. When teaching the officers, David learns to be more patient with people, not to speak over them, and to explain things in a way that they can understand.

*Because as scientists, we tend to speak in very technical terms, very scientific terms, so a lot of times you've got not talk like that, you've got to be able to talk like what we call the layman's way,* *so that people understand what's happening. And then it's just like when you are teaching undergrads, a lot of them just don't care or they just don't understand, and you just have to tell them over and over and over again, or teach them over and over and over again, and it's the same thing here except this time it's not undergrads, they are police officers.* *~David*

**Limitations**

There are a variety of possible career paths for chemistry doctoral graduates; however, this study only focuses a few of them. These participants provided valuable insights into the daily activities and necessary transferable on-job skills in chemistry-related careers. However, the small sample size exerts a limiting effect on the validity of the results. A larger sample size may provide more possibilities of career options and generalizable findings of transferable on-job skills for new chemistry hires.

**Discussions & Implications**

There are many career paths available to chemistry doctoral students. For example, professions include companies in industry, careers in education (teach chemistry in high school, community college or university level), government agencies, and careers related to law (patent attorney, forensic science). In this study, the occupations of these participants include entry-level scientists in industry, teaching-intensive faculty in academia, and scientists in state agencies. These career options provide some possibilities to doctoral students for choosing a job that will fit their best interests.

This study explores careers in chemistry sciences via in-depth interviews with recently hired employees. The semi-structured interview approach can delve into individual experiences and perceptions that provides extensive details about the participants' daily activities. Thus, it is helpful to understand in depth about the profile of chemists in different job sectors. This study is a good resource for doctoral students to get familiar with life in teaching-intensive academic careers and other job sectors, which are not easy to get experience from. The interview summary will help doctoral students have a deeper understanding of the specific career and corresponding job responsibilities. Therefore, this study will help them make better career choices at graduation. Similarly, for chemistry programs that primarily focus on research-intensive trainings, it is beneficial to make chemistry educators aware of other career pathways. It will help them give doctoral students the appropriate advice for choosing a certain career in chemistry.

Our study indicates that doctoral chemists in different job sectors with different job responsibilities require different transferable on-job skills. Depending on the requirements of a specific job, some of the companies in industry or state agencies in government offer on-job training programs to new hires in order to make them well prepared for their jobs. The findings of this study can guide graduate students on what transferable on-job skills they need for each potential pathway, especially when they are freshly hired for a job. The study also indicates that chemistry educators can incorporate some of these transferable skills into the chemistry curriculum. For instance, educators can train doctoral students to engage the community of non-scientists, provide students opportunities to experience industrial settings, and encourage students to speak to the public and explain concepts with clarity. Furthermore, it can guide the faculty in chemistry departments to advise or train doctoral students with some of these skills based on the career paths that students want to pursue after graduation.

This new hire-centered study is a valuable tool for closing the gap between fresh doctoral graduates and employees. To understand the challenges that come with new hires and the current state of their on-job skills will help students be cognizant of what is required for a certain job and prepare for it early in their doctoral programs. By exploring the new hires' views about how they successfully complete daily tasks and overcome challenges in their day-to-day activities helps the institutions know more accurately about possible career development for the new graduates and what skills they require to land a job and to be successful in such a career.

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# CHAPTER 6: A SIMPLE APPROACH FOR BEGINNERS TO DRAWING LEWIS STRUCTURES, RESONANCE FORMS, AND ISOMERS

## Introduction

Lewis structures, also known as electron-dot structures, are diagrams that represent how the electrons are arranged around each atom in a molecule or ion. Drawing Lewis structures is an important skill that students need to acquire in the introductory chemistry curriculum. It is the starting point for understanding and predicting some physical and chemical properties, such as molecular geometry using the Valence Shell Electron Pair Repulsion Theory (VSEPR), acidity and basicity, reactivity, polarity, intermolecular forces, and solubility etc.[1-8]

However, a number of studies found that students had difficulties drawing Lewis structures.[3-6, 9-16] Lever[10] mentioned the confusion about determining the correct number of multiple bonds when students drew a Lewis structure. Additionally, Cooper et. al[16] noted that drawing Lewis structures were more difficult for students in the following circumstances: (a) increased molecular complexity, such as change from one- to two-carbon species, and (b) the formula was presented without structural cues even for some simple molecules.

In order to help students draw Lewis structures correctly and easily, various approaches have appeared in the research literature and general chemistry textbooks.[1-4, 9-15, 17-24]

Lever[10] proposed "6N+2" rule for noncyclic molecules, in which the number of π bonds can be determined by the total number of valence electrons and the total number of atoms in a molecule. Following by this proposed rule, Clark[12] provided detailed procedures for writing Lewis octet structures without understanding s or p bonding. In the same year, Zandler & Talaty[2] listed more examples to account for more types of species, such as cyclic molecules. However, the rule is not applicable to non-octet Lewis structure or odd-electron structure.

Pardo[1] created another method for drawing Lewis structures using the total number of valence electrons and the total number of electrons needed for octet to identify the σ and π bonds. While this approach works well for species that follow the octet (or duet) rule, it is not applicable for hypervalent or incomplete octet molecules. Additionally, students are generally taught Lewis structures prior to really learning what s and p bonds refer to, so delineating bonds as s or p would be conceptually difficult for students.

Similarly, Miller developed guidelines[18] that call for distributing the bonding electrons to atoms to form single bonds or multiple bonds. This is followed by dividing total valence electrons to bonding and nonbonding electrons. Alternative procedures were presented by Mortimer, Davis, Gaily[19], Ahmad & Omar[3], and Whitten[20], these procedures follow the strict octet rule and cannot be applied to free radicals. In addition, the procedures are complicated and require iterative calculations when molecular complexity increases, so that it is likely to make mistakes for beginners when writing the Lewis structures.

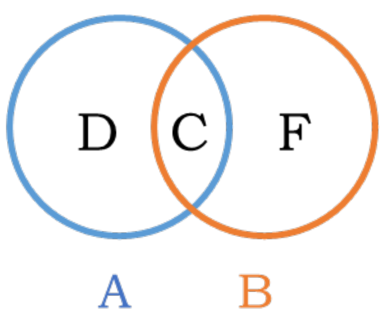
The approach introduced by Carroll[9] requires only the number of valence electrons rather than the octet rule. When drawing a Lewis structure, all electrons are assigned to atoms in pairs to form bonds or lone pairs. He stated that the structure with more bonds or less formal charges tend to be more important. However, it is used only for even-electron molecules. Moreover, the octet rule is a fundamental concept in general chemistry curriculum, it is essential to be taught in the class.

Most recently, an approach was outlined by Nassiff and Czerwinski[4]. They emphasized that students follow the summarized table to find the difference between the number of valence electrons required and the number of valence electrons in the complete octet. The examples they introduced are only molecules or ions with specific $AB_X$ format and strictly following the octet rule.

Some other methods or rules[11, 15, 21-23] either describe simple but inadequate procedures or are too complicated and difficult for beginners to understand. To deal with the difficulties[10, 16] students encountered, a simplified method for drawing Lewis structures, resonance forms, and isomers for molecules or ions is introduced. To expand the use of this method, the adjusted procedures to deal with some of the odd-electron, hypervalent, and incomplete octet molecules or ions are also proposed herein.

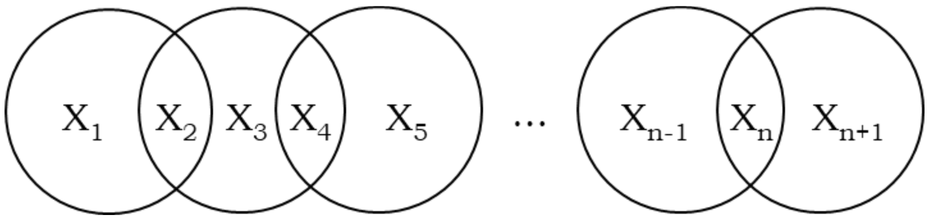
**Rationale**

Assuming that circles A and B represent two datasets, respectively. $C = A \cap B$, is the intersection of these two datasets, and dataset $D = A - C$; $F = B - C$. Thus, $A + B = (D + C) + (F + C) = (D + C + F) + C$.




Thinking about a molecule and its Lewis structure, assume that D and F are nonbonding electrons around atoms A and B, while C is the number of bonding electrons between them. The total number of valence electrons in a molecule is given by D + C + F; the numbers of electrons needed to complete the octet (duet for hydrogen) for each atom are given by D +C and F + C. Thus, the difference between the total electrons needed for the octet and the total valence electrons indicates the number of bonding electrons. As two bonding electrons form one chemical bond, the number of bonds formed by every two electrons can be determined.

The following generalized model for molecules / ions with multiple atoms is provided below to show how one can easily calculate the bond number for the molecule, which is used to determine the number of single, double, and triple bonds in molecules.




Assume the Lewis structure is known and let the number of electrons in a bond be represented by $X_2$, $X_4$... Xn, so that the number of nonbonding electrons in each atom be represented by $X_1$, $X_3$, $X_5$... $X_{n-1}$ and $X_{n+1}$. Under this nomenclature, the total number of valence electrons is determined by Equation (1).

$$\text{Total valence electrons} = X_1 + X_2 + X_3 + X_4 + X_5 + \ldots + X_{n-1} + X_n + X_{n+1} \quad (1)$$

Therefore, the number of electrons needed to complete the octet for each atom is given in Equation (2).

$$= (X_1 + X_2) + (X_2 + X_3) + (X_3 + X_4) + (X_4 + X_5) + \ldots + (X_{n-1} + X_n) + (X_n + X_{n+1}) \quad (2)$$

$$= (X_1 + X_2 + X_3 + X_4 + X_5 + \ldots + X_{n-1} + X_n + X_{n+1}) + (X_2 + X_4 + \ldots + X_n)$$

The difference between Equations (2) and (1) yields the number of bonding electrons (Equation (3)), which easily yields the bond number across the molecule by dividing into two:

$$\text{Bond number} = (X_2 + X_4 + \ldots + X_n)/2 \quad (3)$$

This means that a student can determine the total bond number of the molecule, and therefore how many single, double, and triple bonds are necessary, by knowing only the number of valence electrons and number of electrons needed to complete the octet. A procedure is described below to then work backwards to determine the number of bonds in the molecule.

**Procedures**

**General procedures**

(A). Select an appropriate skeletal atom arrangement for a chemical formula. The atoms, H and F, occupy the peripheral position in any polyatomic molecule or ion. If there are different reasonable atom arrangements, they represent isomers.

(B). Count the total number of valence electrons ($Vale^{-}_{tot}$) in the species by adding together the numbers of valence electrons of each atom as one normally would. For each anion/cation, the number of electrons that equal to the charge should be added/subtracted.

(C). Calculate the total number of electrons needed to theoretically complete the octet ($E_{octet}$) with all the atoms in the molecule or ion by Equation (2). In case of existing hydrogen atoms, two electrons will be added to each of these atoms instead of eight.

$$E_{octet} = 8e^{-} \text{ x } M + 2e^{-} \text{ x } N \text{ ,} \quad (4)$$

where M = the total number of non-hydrogen atoms; N = the total number of hydrogen atoms.

(D). The number of bonding electrons (shared electrons) is determined by subtracting the number of valence electrons from the theoretical needed to complete the octet (equivalent of Equation (3):

$$\text{Bond number} = (E_{octet} - Vale^{-}_{tot}) / 2 \quad (5)$$

(E). List all possible bond number combinations based on the type and the number of peripheral atoms.

$$\text{Bond number} = N + P + A_{M,single} + 2A_{M,double} + 3A_{M,triple} \quad (6)$$

where P is the number of peripheral halogens and $A_{M, single}$, $A_{M, double}$, $A_{M, triple}$ are bond numbers representing the number of single bond(s), double bond(s), and triple bond(s) that exist between

M atoms. Hydrogen and halogen atoms are assumed to form single bonds. For example, the total bond number calculated by procedure (1)-(4) for $C_2H_4O$ is 7. Applying Equation (6), we assume that N = 4 (4 hydrogen), P = 0 (no peripheral halogens), and M = 3 (2 carbon, 1 oxygen):

$$7 = 4 + 0 + A_{M,single} + 2A_{M,double} + 3A_{M,triple} \quad (7)$$

$$3 = A_{M,single} + 2A_{M,double} + 3A_{M,triple}$$

The possible combinations that satisfy Equation (7) are: 3 single bonds ($A_{M,single} = 3$; $A_{M,double} = A_{M,triple} = 0$); 1 single bond and 1 double bond ($A_{M,single} = 1$; $A_{M,double} = 1$; $A_{M,triple} = 0$); and 1 triple bond ($A_{M,single} = A_{M,double} = 0$; $A_{M,triple} = 1$). There must be (M – 1) bonds at this step (each M atom needs to have one bond between them), so having 3 single bonds is not possible nor is having 1 triple bond. The only plausible solution is for the M atoms to contain one single bond and 1 double bond.

(F). Draw the total number of single, double, and triple bonds calculated and complete the octets on each atom (duet on hydrogen) for all the possible structures, which represent different resonance forms.

(G). Check formal charges for those molecules with multiple structures possible.

Odd-electron molecules and expanded / incomplete octet molecules disobey the octet rule. Thus, the adjusted procedures are proposed to handle some of these cases.

**Adjusted procedures for some cases that violate octet rule**

*Radicals*

If the total number of valence electrons is odd, it represents the free radical. All steps are still applicable, with slight modifications to step (D) and (F).

(D). The number of bonding electrons (Equation (6)) is calculated by first subtracting the one radical election before computing the bond number:

$$\text{Bond number} = (E_{octet} - Vale^{-}_{tot} - 1) / 2 \tag{8}$$

(F). Draw the total number of single, double, and triple bonds calculated and complete the octets on all atoms (duet on hydrogen) except one atom filled with the rest of the electrons for all possible structures (last electron will have odd number of electrons).

*Expanded and Incomplete Octets*

If the molecule has only one central atom and the other atoms are peripheral atoms (hydrogen and/or halogens), the procedures introduced here can be used to recognize the expanded or incomplete octets given only the molecular formula of a molecule. Note that so-called expanded octets are contentious in the community and there are better ways to describe and represent the bonding in these molecules, but this method assumes the traditional hypervalent explanation that allows atoms below the second row to have "expanded octets."

A molecule with an expanded octet can be recognized when there is one central atom and the bond number calculated in step (D) is **less than** the number of peripheral atoms (N + P). For example $PF_3$ is not a hypervalent case because the bond number of molecule resulting from (D) is 3 is the same as or greater than the number of peripheral atoms, 3. However, $PF_5$ yields a bond number of 4 which is less than the number of peripheral atoms, 5.

A molecule with an incomplete octet can be recognized when there is one central atom and the bond number calculated in step (D) is **greater than** the number of peripheral atoms (N + P). For example, $BH_3$ yields a bond number of 4, which is greater than the number of peripheral atoms, 3.

In either case, the procedures should disregard step (E) and (H), step (F) will be modified:

(F) Assume a single bond for all peripheral atoms and complete the octets on peripheral atoms, leaving other electrons on the central atom to form M bonds.

**Examples**

The procedures introduced above can be applied to a variety of examples, including diatomic molecules, polyatomic species, complex ions, free radicals, some hypervalent or incomplete octet molecules.

Example 1: $O_2$

(A). Atom arrangement

O O

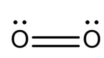
(B). Total number of valence electrons = $6e^-$ (O) x 2 = $12e^-$

(C). The number of total electrons needed to complete the octet =$8e^-$ x 2 = $16e^-$ (M = 2)

(D). Bond number = ($16e^-$ - $12e^-$) / 2 = 2

(E). 2 = 0 + 0 + $A_{M,single}$ + $2A_{M,double}$ + $3A_{M,triple}$ ; 1 double bond is the only possible combination

(F). Draw 1 double bond and complete octets on each atom:



(G). There is only one Lewis structure of $O_2$, skip this step.

Example 2: $CN^-$

(A). Atom arrangement

C N

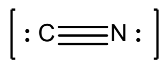
(B). Total number of valence electrons = $4e^-$ (C) + $5e^-$(N) + $1e^-$ (anion) = $10e^-$

(C). The number of total electrons needed to complete the octet = $8e^-$ x 2 = $16e^-$(M = 2)

(D). Bond number = ($16e^-$ - $10e^-$) / 2 = 3

(E). $3 = 0 + 0 + A_{M,single} + 2A_{M,double} + 3A_{M,triple}$ ; 1 triple bond is the only possible combination

(F). Draw 1 double bond and complete octets on each atom:



(G). There is only one Lewis structure of $CN^-$, skip this step.

Example 3: $CO_2$

(A). Atom arrangement

O C O

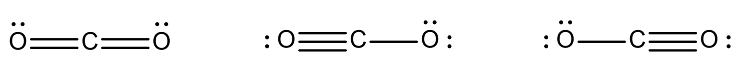
(B). Total number of valence electrons = $4e^-$(C) + $6e^-$ (O) x 2 = $16e^-$

(C). The number of total electrons needed to complete the octet = $8e^-$ x 3 = $24e^-$ (M = 3)

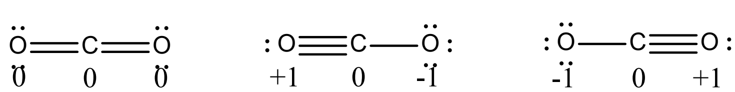
(D). Bond number = $(24e^- - 16e^-) / 2 = 4$

(E). $3 = 0 + 0 + A_{M,single} + 2A_{M,double} + 3A_{M,triple}$ ; possible combinations include 2 double bonds, 1 single bond and 1 tiple bond, and one triple bond and 1 single bond. Therefore, we can expect three resonance forms for $CO_2$.

(F). Draw three structures, one with 2 double bonds and two with 1 single bond and 1 double bond and complete octets on each atom for all the possible structures.

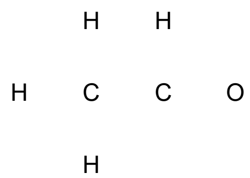


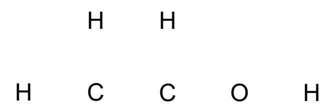
(G). Check for the formal charges on each atom, and the first structure with zeros on all atoms is the best representative for $CO_2$.



Example 4: $C_2H_4O$

(A). Atom arrangement:




There are two reasonable atom arrangement, they indicate two isomers for this chemical formula.

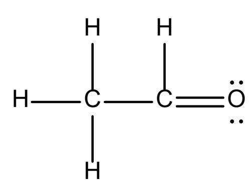
(B). Total number of valence electrons = $4e^-$(C) x 2 + $1e^-$(H) x 4 + $6e^-$(O) = $18e^-$

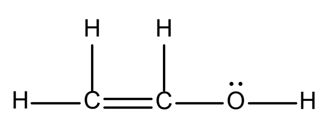
(C). The number of total electrons needed to complete the octet = $8e^-$ x 3 + $2e^-$ x 4 = $32e^-$ (M = 3; N = 4)

(D). Bond number = $14e^-/2$ = 7 bonds

(E). $7 = 4 + 0 + A_{M,single} + 2A_{M,double} + 3A_{M,triple}$, thus $3 = A_{M,single} + 2A_{M,double} + 3A_{M,triple}$; possible combination is only 2 double bonds and 1 single bond. Thus, there should be two forms for $CH_3CHO$.

(F). Draw two structures and complete octets on each atom (duet on hydrogen) for all the possible structures.





(G). The formal charges on all atoms in these two structures all equal to zero, these two structures are isomers.

Example 5: NO

(A). Atom arrangement

N O

(B). Total number of valence electrons = $5e^-(N) + 6e^-(O) = 11e^-$

(C). The number of total electrons needed to complete the octet = $8e^- \times 2 = 16e^-$ (M = 2)

(D). Odd-electron molecule, Bond number = $(16e^- - 11e^- - 1) / 2 = 2$

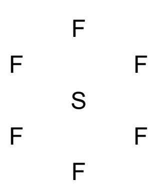
(E). $2 = 0 + 0 + A_{M,single} + 2A_{M,double} + 3A_{M,triple}$; 1 double bond is the only possible combination

(F). Draw two structures each with 1 double bond and complete octet on one atom, leaving the other atom filled with the rest of the electrons (odd number) for all possible structures.

(G). Check for the formal charges on each atom, and the first structure with zeros on both atoms is the best representative for NO.

Example 6: $SF_6$

(A). Atom arrangement



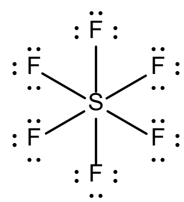
(B). Total number of valence electrons = $6e^-(S) + 7e^-(F) \times 6 = 48e^-$

(C). The number of total electrons needed to complete the octet =$8e^- \times 7 = 56e^-$ (M = 7)

(D). The number of bonding electrons = $(56e^- - 48e^-) /2 = 4$. Because 4 < 6 (M), it indicates that the central atom exhibits an expanded octet.

(E). Skip this step

(F). Draw all single bonds and complete octets on peripheral atoms.



(G). Skip this step.

Example 7: $BeCl_2$

(A). Atom arrangement

Cl Be Cl

(B). Total number of valence electrons = $2e^-$(Be) + $7e^-$ (Cl) x 2 = $16e^-$

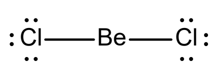
(C). The number of total electrons needed to complete the octet =$8e^-$ x 3 = $24e^-$ (M = 3)

(D). Bond number = $8e^-/2$ = 4 bonds

Since 4 > 2 (M), it indicates that the central atom exhibits an incomplete octet.

(E). Skip this step

(F). Complete octets on peripheral atoms, leaving other electrons on the central atom to form two single bonds.



(G). Skip this step.

**Conclusions**

The method proposed in this paper is simple for beginners to draw an appropriate Lewis structure, its resonance forms, as well as isomers. The algorithm is based on simple calculations and easy to understand for beginners, especially when the molecular complexity increases because the number of multiple bonds in a molecule is easy to be determined by this approach. The approach is the direct application of the octet rule. However, it can also be applied to various species violating the rule, such as some types of odd-electron, hypervalent, incomplete octet molecules or ions. In addition, it does not require σ/π concept prior to Lewis structures, so that students will not have conceptual difficulties when using this method.

The procedures introduced here are expected to provide an alternative to teaching Lewis structures for beginners, but not meant to be exhaustive for all molecules. For example, the central atom sulfur may exhibit an expanded octet to reduce high formal charges in the octet structure of $SO_4^{2-}$. The non-octet structure for $SO_4^{2-}$ cannot be drawn by this proposed method. Other exceptions include $PO_4^{3-}$, $POCl_3$ etc. These non-octet structures remain challenging for teaching using the recent reported methods, as there is no clue for beginners to figure out which is the exception. It would need further studies.

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# CHAPTER 7: CHIRAL

Building Assessment Capacity in Chemistry Education - The Chemistry Instrument Review and Assessment Library (CHIRAL)

## Introduction

Evaluating an educational initiative relies on effective measurements; these measurement data are collected using assessment instruments. The assessment instruments include evaluating aspects of cognitive domains (measures of content knowledge and intellectual skills) or affective domains (measures of emotional and attitudinal engagement with the subject matter) or observational protocols (information on instructor's or student's behaviors). These all require well developed assessments to provide meaningful evidence.

When researchers and educators develop an instrument or use an existing instrument, data should be evaluated for evidence of reliability and validity. To search for an appropriate instrument to use, as a broader community would not be trained in psychometrics much, or some researchers and educators do not have sufficient time and funding to develop an instrument, it is essential to have easy-to-use resources for individuals to understand the validity and reliability evidence. In addition, a consistent peer-review process that summarize the evidence can help users better understand an assessment instrument.

Researchers in STEM fields have developed websites or libraries with searchable instruments, such as he Mathematics Assessment Project (MAP),[1] the Assessing Women and Men in Engineering project (AWE),[2] assessment resources for undergraduate geoscience education.[3] Other libraries go a step further by including evidence of validity and reliability. One example is the library for physics education instruments developed as part of the PhysPort for physics teachers.[4]

Despite the abundance of instrument libraries in STEM fields, only a few contain chemistry education assessment instruments. This CHemistry Instrument Review and Assessment Library (CHIRAL) project aims to develop an assessment library capable of enhancing the evidence used to support instructional practices in chemistry education. It can provide valuable information to chemistry researchers and high school teachers to know the available instruments and related information about the quality of such an instrument. The CHIRAL is designed to contain 1) a searchable database of available inventories which can be filtered according to several parameters (e.g. keywords, domains, specific topics), 2) an overview of the goals, purpose, references, evidence for validity and reliability of the assessment, and other relevant metadata about the assessment, 3) panel-reviews that summarize the existing evidence for validity and reliability of the data produced by the assessment in literature, and 4) a glossary of key terms used frequently in assessment research.

The goal of this study is to identify the participants' current use of evidence-based assessments and the features that would be desired by and/or beneficial to the chemistry education community.

## Methods

### Participants

Faculty members in chemistry departments or high school chemistry educators were invited to participate in an interview conducted via Zoom. The goal of the interview is to identify which features would be desired by and/or beneficial to the chemistry education community by asking questions about the knowledge of assessment terms and concepts, current use of evidence-based assessments, and hypothetical scenarios of how faculty might use a library such as CHIRAL. This interview was about 45 minutes and the research group provided $25 Amazon gift card for each participant's contribution.

We recruited participants from Chemed listserv, NARST listserv, and ChemEd X blog. The goal in recruiting was to interview people with different backgrounds and with a range of interest in research-based assessment. A total of ten participants were interviewed. Among them, there were four chemistry education researchers, four lab coordinator or instructors, two high school teachers. The courses that the participants regularly teach were listed in Table 14. In terms of teaching classrooms, seven participants were teaching in the traditional lecture spaces, while three were teaching in the active learning classrooms. The instructional strategies that they typically use were group work, problem solving, peer learning, flipped classroom etc.

**Table 14. Teaching Background of Participants**

| **Courses** | **Instructional Strategies** |
|---|---|
| organic chemistry (3) | group work (4) |
| general chemistry laboratory (3) | worksheet/solving problems (2) |
| graduate seminar (2) | peer learning (2) |
| college prep classes (1) | iclicker questions (2) |
| general chemistry (1) | guided inquiry (2) |
| science communication (1) | reflection questions (1) |
| introduction to science (1) | cooperative learning (1) |
| introductory biochemistry (1) | partial flipped classroom (1) |
| accelerated chemistry (1) | 100% flipped classroom (1) |
| academic chemistry (1) | interdisciplinary lessons (1) |

| | |
|---|---|
| | semi-interactive lecturing (1) |

### Data collection

The interview protocol was designed to include four parts. The first part was the participants' background information collection, the participants were asked about their primary responsibilities and their roles, the classes they were teaching, the classroom spaces they were using for a regular class, and their instructional strategies. The second part was their current use of the evidence-based assessment. They were asked about the assessments they were using, the resources to find an assessment, the assessment quality evaluation, and result analysis. The third part was the needs assessment. The participants mentioned the valuable features they desired, their potential use of the resource, and the necessity of panel summary and glossary. The last part was the suggestions that the participant gave to us, such as their preference of mobile device, and their thoughts on the site mock-up image. See Appendix 11 for interview protocol.

## Results

### Participants' current use of the evidence-based assessment

There were seven participants using evidence-based assessments in their classrooms. The specific assessments that the participants were using include ACS exam, evaluating the understanding of periodic table assessment, chemistry concept inventory, ASCv2(Attitudes towards Subject of Chemistry), self-efficacy assessment, scientific literacy skill assessment, biochemistry concept inventory, acid-base chemistry inventory, ALEKS, and the exams they wrote on their own. Among them, self -efficacy and scientific literacy skill assessments are general assessments, others are chemistry-specific. When the participants were searching for an assessment, they would like to find one from resources such as ACS exam, study guide for ACS exam, online test bank, *Next Generation Standard*, *Common Core Standards*, *AAAS Science Assessment*, content of concept inventory, Dr. Bretz's website regarding assessment resources, chemistry education community, NARST listserv, *Journal of Chemical Education* (JCE) articles; conference, and workshop.

When they considered implementing an assessment, all but one said that they paid attention to evidence of validity and reliability to evaluate the quality of an assessment. Additionally, they mentioned others points for evaluating the quality of an assessment. For example, how well the assessment aligns with the course, how clear the question is, whether the result can compare to the national data, how long it will take to administer the instrument, the representational level of target sample, difficulty of the questions, and whether the assessment can test students' ability to process information.

Participants mentioned several approaches to analyzing the results of the assessments. They like to compare the results with the national norms, such as comparing to ACS national level performance on specific topic, comparing to national level data in general, comparing the results with ones presented in national or local conferences. Other analysis included calculating average gain score, using learning analytics tool OnTask to analyze students' overall performance.

Unlike these seven participants, the other three participants did not use evidence-based assessments in their classrooms. Reasons include difficult to find or non-existent assessments and how the assessment fits into their own courses. If they were to look for an evidence-based assessment, the participants would look for one in Google Scholar, ACS publications website, journal articles, chemistry education community, and conferences. These resources are similar as those responded by the participants that were using the assessments in the classrooms.

Even though they were not using evidence-based assessments, they mentioned the importance of validity and reliability when they thought about implementing an assessment in the class. In addition, they would pay attention to how well an assessment aligns with the course, the assessment's standards and goals, whether it can meet the students' needs, and the assessment is formative or summative. If they were to analyze the results, they would perform factor analysis to gather evidence of validity; compare to the results in the context of what the students have done in prior study and give feedbacks to the students.

Among these ten participants, there were four chemistry education researchers. They were asked about the evidence they collected to support the validity and reliability of the assessment for their research project or in their classrooms. The evidence they gathered to demonstrate the validity included concurrent validity, predictable validity, face validity, convergent and divergent validity, expert reviews (evidence based on test content), student interview (evidence based on response process), factor analysis (evidence based on internal structure), compared to other concept inventory that exist (evidence based on relation to external variables). The reliability evidence they collected included Cronbach' α for continuous variables and split-half reliability. The approaches of how they dealt with the results were give feedbacks to the students based on the results, updating the test / making improvements, and using them as research tools.

**Needs assessment**

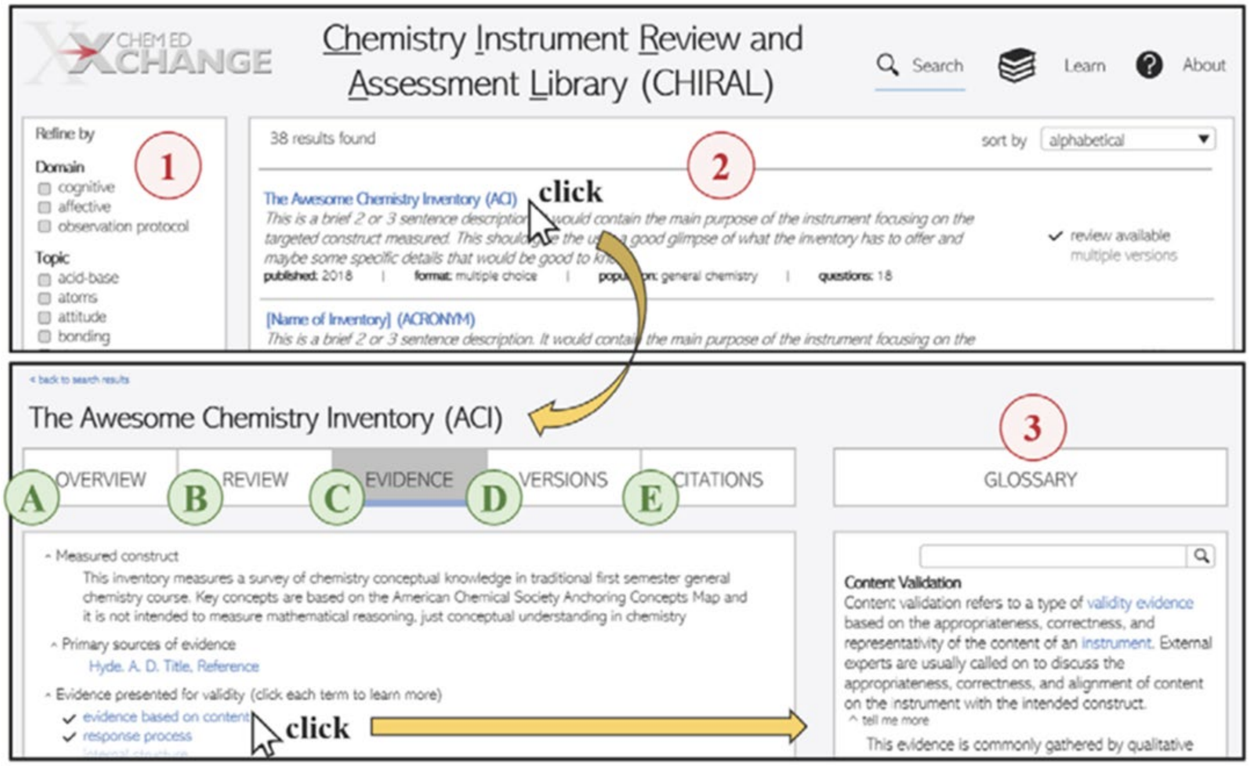
In this part, the participants were asked about the planned features and the additional features they would find valuable both to them personally in their teaching (and research if applicable) as well as to the broader chemistry education community. They responded with a variety of features, most of them would like to have access to assessment items and can compare their data with national norms. Specifically, they would like to have the display of items, the number of items, the information of item format (open-ended or multiple choices). Additionally, they cared about the quality of assessment, the evidence of validity and reliability. Some of them preferred to have the details of the evidence, while others preferred to have a simple star rating and brief summary of the validity and reliability evidence. Some other features that participants find valuable included the big picture of the CHIRAL project, the inventory title and objectives, authors' information to connect with, representational level, chemistry division, time of administration, possible application of an assessment, references, searchable topic-based list, best practices, editable / customizable remarks, information of difficulty and discrimination.

Their potential use of CHIRAL website included searching for an assessment, constructing assessments, systematic reviews, identifying gap between the published studies and what can be studied in the future, contributing back to this site, knowing students' misconceptions, using assessments in their class, suggesting inventories to others, identifying problems before making changes, departmental discussion about broader curricular issues, and decision making across classes.

**Participants' perceptions of the mock-up of CHIRAL site**

Lastly, the participants were asked to identify how well the mock-up of the CHIRAL site aligned with the features that they were interested in. In Figure 16, Part 1 shows a catalog which is searchable and browsable by keywords, domains, specific topics, and other pertinent information. Part 2 contains various information of an instrument, such as name of the inventory, publication date, number of items. For each instrument, a brief summary about the instrument will be displayed on the main search results page. Expanding the record for each instrument will make five tabs available: (A) an overview summarizing instrument metadata and the development history; (B) a peer review panel summary of the available evidence for validity and reliability; (C) validity and reliability evidence presented for data collected using the instrument; (D) alternative versions and translations of the instrument; and (E) citations of published literature utilizing this instrument. Part 3 is the searchable glossary, the entire page will be indexed so that every time a term or concept appears that may be unfamiliar to the user, user can click it and gain access to an in-page glossary that defines this term in varying levels of detail. For Part 1 in **Figure 16**, a manageable list of topics was suggested. Additionally, two participants mentioned that refined by domain was highly theoretical language and was hard to understand. Several participants preferred to have "filter by level" option on the site (e.g. undergraduate vs. graduate; 1st year vs. 2nd year). For Part 2, suggestions included having time to complete the assessment, ranking of the validity and reliability evidence, and Spanish version. For Part 3, participants would like to have independent search bar for glossary. Furthermore, participants suggested to build a community on the site including user's page, results page and data page.

**Figure 16. Mock-up of CHIRAL Site**




## Conclusions

This study identified the participants' current use of the evidence-based assessments and the features that they would find valuable both to them personally in their teaching (and research if applicable) as well as to the broader chemistry education community. It is clear that chemistry researchers and educators value the evidence of validity and reliability of the assessments when they considered implementing them. They would like to have access to the assessment items and can compare the results with national norms. This study also identified how well the mock-up of the CHIRAL site aligned with the features that the participants were interested in. The interviews provided valuable information about the desired features to ensure that the CHIRAL website contains features, information, and tools that the chemistry education community finds useful.

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## Appendix 11: Interview protocol

1. Background

(1) What are your primary responsibilities at your school/university?

(2) Would you characterize yourself as a researcher?

   a. If yes, what type of researcher are you? (e.g. synthetic organic chemist, spectroscopist, chemical education researcher)

(3) What courses do you regularly teach? How big are your classes?

(4) How would you describe your classroom space? (traditional lecture spaces or active learning classrooms)

(5) How would you describe your instructional strategies?

2. Assessment

Current Use of Assessment

(1) What does evidence-based assessment mean to you?

(2) What do validity and reliability mean to you?

(3) Do you use any evidenced-based assessments in your classroom currently?

(4) **If yes**…

   a. Are they generally chemistry-specific or are they more general (like a motivation assessment, for example)?

   b. Can you recall specific assessment names that you use?

   c. What evidence-based assessment(s) do you use *in your class*?

   d. Where and how did you find an assessment?

   e. What do you consider when choosing to implement an assessment you find online?

      i. How do you evaluate the assessment?

ii. Do you pay attention to an assessment's validity and reliability when you use it?

f. What do you do with the results / how do you analyze them?

   i. Have you ever compared your assessment results to other results?

g. Are you satisfied with the conclusions you are able to draw from your current assessments?

**If no…**

h. Are there any specific reasons why you do not use any evidence-based assessments in your classroom? (This is perfectly fine and we are not judging you in anyway, we are just curious.)

i. If you were to look for an evidence-based assessment, where would you look for one?

j. How would you consider implementing an assessment you find online?

   i. How would you evaluate the assessment?

   ii. Would you pay attention to an assessment's validity and reliability when you use it?

k. What would you do with the results / how would you analyze them?

   i. Would you compare your assessment results to other results?

(5) If participant identifies as a chem ed researcher…

a. Do any of your responses change if you think about finding and implementing an assessment for a research project instead of your classroom?

   i. Followups: more/less emphasis on validity, evidence to support it, what to do with the results

Needs Assessment

This interview is part of an NSF funded project that seeks to build a resource that will gather information publicly available about assessments used by the chemistry education community. We are designing this site to contain:

- A searchable database of available inventories which can be filtered according to several parameters
- An overview of the goals, purpose, references, evidence for validity and reliability of the assessment, and other relevant metadata about the assessment
- Panel-reviews that summarize the existing evidence for validity and reliability of the data produced by the assessment in literature
- A glossary of key terms used frequently in assessment research

The next series of questions will ask about the planned features and what additional features you would find valuable both to you personally in your teaching (and research if applicable) as well as to the broader chemistry education community (referred to as "the community").

(1) When considering an inventory, what information would you or the community like available to you right away in a convenient location? (If no response initially, give hints of name of inventory, authors, publication date, number of items, etc.)

(2) What features would you or the community find the most helpful in a site like the one described? Why?

(3) Assuming you had adequate time, how would you or the community potentially use this resource?

(4) What specific things would you or the community like to know about an assessment; what information would you or the community need to make the most informed-decision possible?

(5) If given a summary of the evidence for validity and reliability via a panel summary, do you think you would consider these in your judgement of the quality of an assessment?

   a. Followup: Do you feel that, with the assistance of a glossary and panel-summaries, you would have the requisite expertise to make an informed-decision?

   b. Followup: How familiar are you with the evidence that supports test validity/reliability? Could you provide some details that you would look for to gauge the data of an assessment's validity and/or reliability?

   c. Same questions for the community this time

(6) Would you or the community imagine using a site like this on a mobile device?

(7) Overall, do you think a resource like this would be useful to yourself and the community?

(8) We have created a mock-up of the site and are interested in how well this aligns with what features were important to you. Can you identify features you do and don't like on this image?

3. Others

(1) Do you have any final comments about how we should go about designing/developing this site? Is there anything else we should have asked about but didn't?