Supplementary Information

Doctoral Education in Chemistry: Faculty perspectives on programmatic elements' goals and outcomes

Benedicta Donkor, Melissa A. Collini and Jordan Harshman

Department of Chemistry & Biochemistry, Auburn University, Auburn, Alabama 36849, United States
Corresponding author email address: jharshman@auburn.edu

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Goals and Outcomes Tables

Table S1. Codebook on the codes and definition to the primary goals and outcomes of the individual programmatic elements.

Code	Description
Goals of Elements	Describing goals of individual elements, i.e. responses to what is the goal of the individual programmatic elements.
Goal itself	Responses to "what is/are the goals of the individual programmatic elements?"
Actually get	Responses to "what do students actually gain from the individual programmatic elements?"
Advisor accountability	Keep the advisor from negatively harming students, provide checks and balances on their power over students, extra set of eyes watching, they become your defense against the dark arts, vouch for them
Advisor or Lab pairing	Exposure to a PI before they actually join a research group, allow students to get exposure to a different people, different potential mentors, select an advisor, or the advisor chooses a student, the advisor gets a chance to see the students.
Affective outcomes	To gain an appreciation, confidence, emotional growth, satisfaction, self-confidence and pride, excitement, empathy (they will judge professors less harshly because they themselves are being judged at the same time), get happy, motivate them, interest, gains understanding of what effort it takes to produce and validate new results, persistence, perseverance, resilience, recognition, not to be ashamed of my accent
Career preparation	Preparation for their career, develop a career, essential skill for employment, serve the vocational skill, training students so that they will have options, mentoring students into teaching careers, develop skills and knowledge and abilities and ways of reasoning that would be productive in their careers, it prepares for a huge variety of career path, put on their CV to get an academic job, get the experience that they can put on a resume, getting a letter of recommendation, need other references
Celebratory fanfare	Celebration, fanfare

Communication skills	Communication, being able to write, to be able to summarize the work, to put all research together, present work, the ability to converse on a topic at a high level, giving presentations, practice talks, speaking at a public lecture, discuss research, oral talk, outreach opportunities (science communication, more informal)
Critical or Independent thinking	Contributing their own ideas, think independently, able to synthesize this information together, independent thought, to develop their critical thinking skills, think for themselves, answer questions from curious people, they have to be able to not just doing experiment but what does it mean and what does it mean to have next steps and what can you propose to advance the area, to critique papers, develop independence in research, grow on their own, taking more ownership of the project and contributing their own ideas, feel a sense of ownership of the project, independent scientist, lead projects later on, you learn things well when you teach it, self-learners
Ethics	Discus ethical issue, discussion on general ethical issue, train them in rigor and ethics in doing research
Evaluation and feedback	Evaluation, get feedback, to keep the student on track, review everything that they've accomplished, self-reflection. Communicating expectations to the student.
Free food	Free food
Help faculty or department	They can get tenure, to help their (faculty) own research succeeds, to help the undergraduates, make our jobs sort of easier at the university, cheap labor, to save money, make sure NSF and NIH and other agencies are happy.
Technical knowledge	To gain a body of knowledge, to know the status of the field, the language of the field, to lay the foundation of knowledge, breadth of knowledge, foundational and fundamental chemical knowledge, knowledge base, depth of knowledge, technical knowledge, searching the literature for assistance in either designing experiments, get exposed to science outside of

	their specific research interests, to expose them to other people's work, expertise-deep grounding of own area of research,
Mentorship	Mentor, mentoring skill, mentorship, guiding them as they learn, help the student, give direction, guides them, gain the advice and support, some level a cheerleader, moral support, become role models, having them there as a sounding board, venting off frustrations, maybe within mentorship, but someone/a committee who is primarily responsible for the students' progress, someone that's held accountable for all this stuff. If it mentions specific skills for them to learn we put that in the other goals codes
Networking and Collaboration	Interconnect with each other, to know what everybody in the lab are doing, to learn from other people, to get various kinds of experts deeply engaged, to get exposure to a different people, collegiality, be able to mitigate people disgruntle, to work with the other students in the lab, how different people's projects interconnect with each other, if collaborations are specifically mentioned, establishing collaborations, interdisciplinary teams, Working with others
Novel or significant research	New knowledge they've developed as a result of their efforts, proposing new ones, developing new technologies, creating new knowledge, co-inventor, developing a new methodology or developing a new different technique, creating new knowledge, formulate new ideas and concepts on the fly, engaging in creative activities, to make their own mark on science, very high-impact work. Move an area forward, push the limits of science.
Personal resources	Funding, money, stipend, salary, pay tuition
Planning or organizational skills	Organizational skills, prepare themselves and documents, plans for the completion of their Ph.D., they're organizing a seminar, planning, developing, or designing an experiment, time management skill, learn some structure from that, multitasking
Problem-solving skills	To solve problems, solve problems, problem solving skills, address some gap, to address scientific questions

Research resources	Support of extramural funding that is required to make the research go, space for research, funding, funding for research
Scholarly record	It leaves a permanent record of the work, serves the function of providing tangible evidence, it puts a nice bow on it, Ph.D. level research document, getting publications.
Stress or harm mental health	Just stress and a lost Saturday morning, torture students psychologically, students see it as a hurdle
Supplement advisor	add secondary kind of research advice for what they're doing, get second opinion about their research
Teaching skills	To give them experience in teaching, learn how to teach, to explain to somebody else, and teaching oneself, independent learner
Technical research skills	Formulating or defining a problem, designing experiments, executing experiments, interpreting experiments, pivoting or revising experiments based on outcomes, identifying patterns, identifying new strategies, having students do research, to engage in research, discover how slowly things go in some fields and how fast in other fields activity, Interpret the data, gain practical experience. "How science is done" -counts for Research. If they are talking from mentor perspective, it is mentorship.
Uniform level	To bring them up to a uniform level across the cohort, harmonize everybody's background, fill in gaps from their undergraduate education
Weed Out	to remove bad students, like a weeding out, to ensure some quality control in the people that make it to the end of our program, checkpoint for ensuring that they're going to meet that standard
Workable environment	Advisors create an environment where it's a good learning environment, a good lab environment, build a team and make it work, whether they feel comfortable in a group or lab. Not creating an opportunity for research necessarily but creating a positive environment.

Table S2. Number of faculty who responded to "goal – what is the primary goal of the programmatic elements" and "outcome – what do students actually gain from the programmatic elements" along with the respective percentage to the total number of participants interviewed.

Programmatic Elements	**Goals**	**Percentage out of the 45 Participants (%Goals)**	**Outcomes**	**Percentage out of the 45 Participants (%Outcomes)**
Advisor	37	82.22	23	51.11
Advisory Committee	30	66.67	9	20.00
Annual Evaluation	23	51.11	13	28.89
Candidacy Process	32	71.11	16	35.56
Coursework	34	75.56	22	48. 89
Dissertation and Defense	32	71.11	13	28. 89
Group meetings	34	75.56	11	24.44
Lab rotation	20	44.44	13	28.89
Publication	17	37.78	15	33.33
Research	44	97.78	39	86.67
Seminar	28	62.22	16	35.56
Teaching Assistantship	32	71.11	18	40.00

Table S3. Faculty that were explicitly asked about both the primary goals and outcomes of the individual programmatic elements.

Goals and Outcomes	Programmatic Elements											
	RS (39)	**AD (23)**	**PB (15)**	**GM (11)**	**CE (16)**	**CW (22)**	**DD (13)**	**LR (13)**	**AC (9)**	**AE (13)**	**SM (16)**	**TA (18)**
Technical Research Skills	46		13			14						6
Critical or Independent thinking	38	4	7	9	19					8		6
Technical Knowledge	21	4	7	36	6	86	8				50	28
Novel or significant research	21	4										
Communication skills	18		60	36	19		46			8	50	33
Career Preparation	15	9	27			5			11	8		17
Planning or organizational skills	13		13		13		8				6	6
Problem-solving skills	10			9	6							6
Mentorship	5	91		18					67	23	6	11
Personal resources	3	13										33
Research resources	3	26										6
Networking and Collaboration	3	4		18							13	
Scholarly record	3		20				8					
Teaching skills		4										28
Affective outcomes										8		6
Evaluation and feedback		4	7	45	19		8		22	69	6	
Stress or harm mental health					6						6	
Supplement advisor		4							33			
Advisor Accountability									22			
Advisor or Lab Pairing								100				
Workable environment		4						8				
Uniform level						5						
Celabratory fanfare												
Ethics												
Free food												
Help faculty or department												
Weed Out												

* The goals and outcomes in this table is sorted by the highest percentage of participants that mentioned same goals and outcomes for **research**. Numbers are the percentages of faculty who responded to both questions rounded to the nearest whole number.
RS – **Research, AD – **Advisor**, PB – **Publications**, GM – **Group meeting**, CE – **Candidacy process**, CW – **Coursework**, DD – **Dissertation and Defense**, LR – **Lab rotations**, AC – **Advisory committee**, AE – **Annual evaluation**, SM - **Seminar**, TA – **Teaching assistantship**. The elements are sorted based on faculty rating of their relative importance. The numbers in () represents the total number of faculty explicitly asked both questions.

Appendix A. Method (additional)

Development of Interview protocol

In the first round, BD and MAC conducted interviews with a cohort of 7 participants. Subsequently, an interim halt was introduced in the interview process to facilitate the development of a codebook and to identify any necessary refinements to the interview protocol. Following an initial analysis of these 7 interviews, minor adjustments were made to the interview protocol, involving the reordering of certain questions and enhancing question clarity. For the second round of interviews, involving 12 participants, BD and MAC employed the refined interview protocol. The interview was paused, and data analyzed. The interview protocol was adjusted to prioritize the discussion of programmatic elements that had received comparatively less attention, positioning them at the onset of the interview for the remaining interviews. Notably, programmatic element, research was addressed first, irrespective of the number of participants who had previously discussed it, given its status as the most pivotal programmatic element.

Codebook Development/Data Analysis

Codes similar in definition were combined. For example, the mentorship code encompasses two different types of mentorship. The initial one is students receiving mentorship (where faculty are guiding, mentoring, advising or helping students) while the second is students giving mentorship (where faculty train students to become mentors). However, these two codes were combined as they were all forms of mentorship. Other codes combined were collegiality and networking which were all combined into the networking code. The collegiality code comprised of collegiality, working with other students in the lab, being able to mitigate people disgruntle, etc. while networking was more of interacting with others (colleagues or professors), and getting exposed to other people. The two codes were similar in the sense that they were about students interacting in one way or the other with people inside and outside of their field, hence, combined.

In comparison of the goals and outcomes identified in this study to literature, we identified 12 workforce skills; nine were found to be represented almost exactly in the name of the code and the definition identified by BD and MAC and the remaining three were found to be represented, at least in part, by other codes. For instance, personal attributes from the previous study[11] were partially covered by affective outcomes in this study, while collaboration skills and networking were combined in our study. Management skills in the previous study aligned more with the mentorship component, where students learn to mentor others (in our study). The personal growth and development of the previous study better aligned with aspects of our evaluation and feedback, along with some part of critical or independent thinking (becoming independent part). Organizational awareness aligned with the career preparation and ethics in this study. Therefore, we replaced these skills with corresponding goals and outcomes from our study that better match the workforce skills identified in the previous study[11] as shown in **Figure 2**.

Participant Selection

For the recruitment of participants, we followed a random sampling method across various strata to ensure a diverse representation of chemistry doctoral programs throughout

different regions of the United States. We compiled a comprehensive list of the 202 chemistry doctoral programs in the U.S., which were then categorized into five geographic regions: Northeast, Southwest, West, Midwest, and Southeast. We aimed to gather a sample of faculty that reflected a broad range of personal identities (including race and gender) and academic identities (such as area of interest, university affiliation, and academic rank). Following 19 interviews, we evaluated the distribution of participants concerning personal and academic identities to identify underrepresented groups in our sample, ensuring that diverse perspectives from all demographics were acknowledged and included.