In the Mix Surveys

Pre-In the Mix Questionnaire: Participants

What is your expected graduation year?

- o 2023
- o 2024
- o 2025
- o 2026
- o 2027

How much experience do you have in scientific research?

- o No experience
- o A little experience
- o Moderate experience
- o Considerable experience

Are you currently working on the D3TaLES research project?

- o Yes

- o No
- o Not sure

What is the primary reason you chose to participate in In The Mix?

In a couple of sentences, how would you describe your understanding of connections among computational techniques, data science, and wet-lab experiments?

How much experience have you had **generating** large datasets in research?

- o No experience
- o Little experience
- o Moderate experience
- o Considerable experience

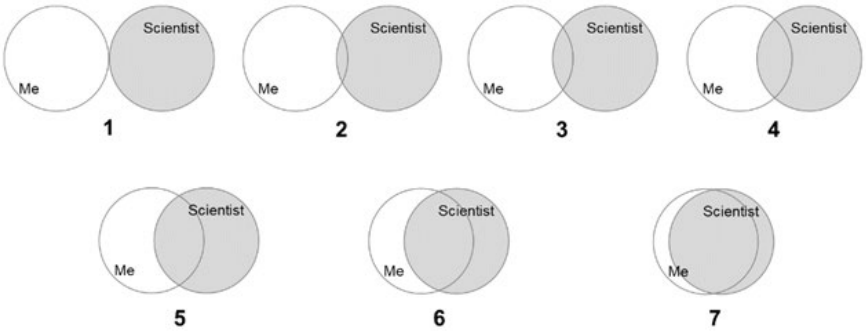
How much experience have you had **utilizing** large datasets in research?

- o No experience
- o Little experience
- o Moderate experience
- o Considerable experience

Which numbered picture best describes the current overlap of the image you have of yourself with that of a scientist?

- o 1
- o 2
- o 3
- o 4

- o 5
- o 6
- o 7



Pre-In the Mix Questionnaire: Graduate Student Leaders

Which group(s) are you helping to lead for In the Mix 2023?

1. Computational
2. Machine Learning
3. Electrochemistry

How much experience, if any, did you have designing teaching activities prior to designing activities for In the Mix 2023?

- o None
- o A little
- o Some
- o A lot

Thinking about preparation for In the Mix 2023, would you say you are behind where you expected to be, about where you expected to be, or ahead of where you expected to be?

- o Behind expectations
- o About as expected
- o Ahead of expectations

Considering your previous experience and preparation to this point, how effective do you think you will be in leading activities at In the Mix 2023?

- o Not at all effective
- o Slightly effective
- o Somewhat effective
- o Very effective
- o Not sure

What has gone better than expected with In the Mix 2023 planning?

What has not gone as well as expected with In the Mix 2023 planning?

What have been the greatest challenges, if any, with planning In the Mix 2023?

What is your most valuable takeaway from planning In the Mix 2023?

Please note any additional comments that you would like to share about In the Mix 2023 planning, structure, or content.

Post-In the Mix Questionnaire: Participants

Which day(s) did you attend In the Mix?

- o Thursday only
- o Friday only
- o Both Thursday and Friday

Overall, how would you rate the *In the Mix* workshop?

- o Poor
- o Fair
- o Good
- o Excellent

What would you say was the most valuable content or experience? Please enter a phrase or two.

What did you find least valuable?

How much, if at all, do you think your participation in *In the Mix* has improved your research skills?

- o Very little or no improvement
- o Slight improvement
- o Substantial improvement
- o Major improvement

How would you describe any shifts in your understanding of connections among computational techniques, data science, and wet-lab experiments after participating in *In the Mix*?

In a couple of sentences, please describe your current understanding of the role of large datasets in research.

Please indicate how much you agree or disagree with each statement. By transdisciplinary, we mean research efforts conducted by investigators from different disciplines working jointly to create new conceptual, theoretical, methodological, and translational innovations that integrate and move beyond discipline-specific approaches to address a common problem.

	Strongly agree	Somewhat agree	Neither agree nor disagree	Somewhat disagree	Strongly disagree
I would describe myself as someone who strongly values transdisciplinary collaboration	o	o	o	o	o
Transdisciplinary research interferes with the ability to maintain knowledge in your primary area	o	o	o	o	o
I tend to be more productive working on my own rather than working as a member of a transdisciplinary research team	o	o	o	o	o
Transdisciplinary research stimulates me to change my thinking	o	o	o	o	o
Transdisciplinary research will improve how I conduct research	o	o	o	o	o

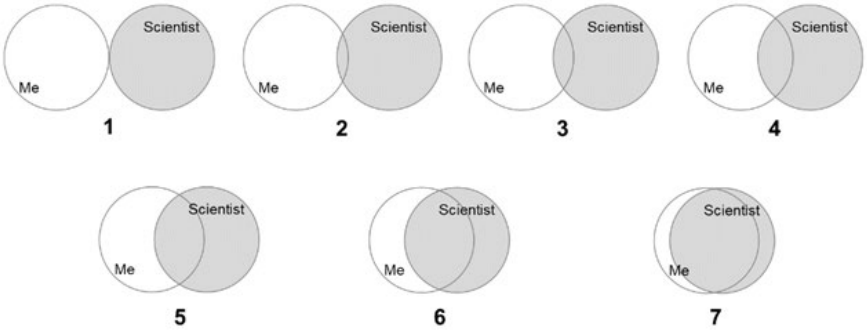
I am optimistic that transdisciplinary research among participants will lead to valuable scientific outcomes that would not have occurred without that kind of collaboration	o	o	o	o	o
Because of my involvement in In the Mix, I have an increased understanding of what my own discipline brings to others	o	o	o	o	o
Generally speaking, I believe that the benefits of transdisciplinary scientific research outweigh the inconveniences and costs of such work	o	o	o	o	o
I am comfortable working in a transdisciplinary environment	o	o	o	o	o
Overall, I am pleased with the effort I have made to engage in the In the Mix program	o	o	o	o	o

Which numbered picture best describes the current overlap of the image you have of yourself with that of a scientist?

- o 1
- o 2
- o 3
- o 4
- o 5

o 6

o 7



Please indicate whether you think there was not enough time, enough time, or too much time spent on the following Day 1 activities:

	Not enough time	Just the right amount of time	Too much time	Don't know/Not sure
Motivation & Background	o	o	o	o
Computational, Part 1	o	o	o	o
Machine Learning, Part 1	o	o	o	o
Tour	o	o	o	o

Please indicate whether you think there was not enough time, enough time, or too much time spent on the following Day 2 activities:

	Not enough time	Just the right amount of time	Too much time	Don't know/Not sure
Electrochemistry, Part 1	o	o	o	o
Electrochemistry, Part 2	o	o	o	o
Computational, Part 2	o	o	o	o
Machine Learning, Part 2	o	o	o	o

Please indicate your level of understanding related to the following computational activities.

	Understand very little	Understand somewhat	Understand fairly well	Understand very well
How DFT works	o	o	o	o
How to build molecular structures	o	o	o	o
Performing a geometry optimization	o	o	o	o
Viewing the HOMO and LUMO of the optimized molecule	o	o	o	o
Calculating redox potentials using the Born-Haber cycle	o	o	o	o
Correlations between HOMO/LUMO and oxidation/reduction potential	o	o	o	o

Please indicate your level of understanding related to the following experimental activities.

	Understand very little	Understand somewhat	Understand fairly well	Understand very well
Setting up electrochemical cell	o	o	o	o
Acquiring CV	o	o	o	o
Analyzing CV	o	o	o	o
Peak splitting	o	o	o	o
Comparison to computational outcome	o	o	o	o
Connecting e-chem outcome back to chemical structure	o	o	o	o
Safety & chemical hygiene	o	o	o	o
Reproducibility of data	o	o	o	o

Please indicate your level of understanding related to the following machine learning activities.

	Understand very little	Understand somewhat	Understand fairly well	Understand very well
Data handling using python	o	o	o	o
Data visualization using python	o	o	o	o
Basics of machine learning	o	o	o	o
Utilities and challenges of deep learning	o	o	o	o

What *In the Mix* activity did you find most exciting/rewarding? Please describe why.

What *In the Mix* activity or activities did you struggle with the most? Please describe why.

How likely or unlikely are you to recommend *In the Mix* to a friend or classmate?

- o Very unlikely
- o Somewhat unlikely
- o Somewhat likely
- o Very likely

If you were to add or change one thing about *In the Mix*, what would it be, and why?

Post-In the Mix Questionnaire: Graduate Student Leaders

Which group did you help lead for In the Mix 2023?

4. Computational
5. Machine Learning
6. Electrochemistry

Overall, did In the Mix 2023 fall short of, meet, or exceed your expectations?

- o Fell short of my expectations
- o Met my expectations
- o Exceeded my expectations

[If fell short] In what ways did In the Mix 2023 *fall short of* your expectations?

[If exceeded] In what ways did In the Mix 2023 *exceed* your expectations?

How effective do you think you were in leading activities at In the Mix 2023?

- o Not at all effective
- o Slightly effective
- o Somewhat effective
- o Very effective
- o Not sure

For each of the following Day 1 topics and activities, do you think that there was not enough time, just the right amount of time, or too much time allotted?

	Not enough time	Just the right amount of time	Too much time	Don't know/Not sure
Motivation & Background	o	o	o	o
Computational, Part 1	o	o	o	o
Machine Learning, Part 1	o	o	o	o
Tour	o	o	o	o

For each of the following Day 2 topics and activities, do you think that there was not enough time allotted, just the right amount of time allotted, or too much time allotted?

	Not enough time	Just the right amount of time	Too much time	Don't know/Not sure
Electrochemistry, Part 1	o	o	o	o
Electrochemistry, Part 2	o	o	o	o

Computational, Part 2	o	o	o	o
Machine Learning, Part 2	o	o	o	o

For each of the following topic areas included in the In the Mix 2023 schedule, do you think there was not enough depth, just the right amount of depth, or too much depth for participating students?

	Not enough depth	Just the right amount of depth	Too much depth	Don't know/Not sure
Computational	o	o	o	o
Machine Learning	o	o	o	o
Electrochemistry	o	o	o	o

Did you complete the Electrochemistry sessions as a participant?

- o Yes
- o No

Please indicate your level of understanding related to the following experimental activities.

	Understand very little	Understand somewhat	Understand fairly well	Understand very well
Setting up electrochemical cell	o	o	o	o
Acquiring CV	o	o	o	o
Analyzing CV	o	o	o	o
Peak splitting	o	o	o	o

Comparison to computational outcome	o	o	o	o
Connecting e-chem outcome back to chemical structure	o	o	o	o
Safety & chemical hygiene	o	o	o	o
Reproducibility of data	o	o	o	o

Did you complete the Computational sessions as a participant?

- o Yes
- o No

Please indicate your level of understanding related to the following computational activities.

	Understand very little	Understand somewhat	Understand fairly well	Understand very well
How DFT works	o	o	o	o
How to build molecular structures	o	o	o	o
Performing a geometry optimization	o	o	o	o
Viewing the HOMO and LUMO of the optimized molecule	o	o	o	o
Calculating redox potentials using the Born-Haber cycle	o	o	o	o
Correlations between HOMO/LUMO and oxidation/reduction potential	o	o	o	o

Did you complete the Machine Learning sessions as a participant?

- o Yes
- o No

Please indicate your level of understanding related to the following machine learning activities.

	Understand very little	Understand somewhat	Understand fairly well	Understand very well
Data handling using python	o	o	o	o
Data visualization using python	o	o	o	o
Basics of machine learning	o	o	o	o
Utilities and challenges of deep learning	o	o	o	o

If you were to add or change one thing about In the Mix 2023 implementation, structure, or content, what would it be, and why?