Case Study 1: Below the Surface of Surface Chemistry Dr. ChoGlueck

Taylor is a PhD candidate in chemical engineering, who researches thermal reaction rates on metal surfaces. She needs to defend her dissertation by the end of the summer before her new postdoc position begins in the fall. Throughout this spring and summer, she has completed several experiments, with the goal of finding publishable rate constants for hydrogen atoms on platinum surfaces used industrially. Her PhD advisor guided her toward this topic, saying that physical chemists have estimates from theory but lack validation from reliable measurements at actual physical surfaces from well-replicated experiments. She has spent the past two years learning how to create different computer models using different theories to make predictions, with the ultimate goal of validating these simulations experimentally.

Her initial experiments #1, #2, and #3 are fairly promising, and then experiments #4 and #5 are near exact replications of the simulations. Taylor and her advisor are very pleased, and she starts drafting the manuscript and creating the figures as she completes the final experiment—which she considers culmination of her dissertation. Around this time, her advisor leaves for his remote summer home in the mountains, where he only has cell reception for weekly check-ins. He tells Taylor that he trusts her to finish the remaining work and writing. He also says her findings will lead to multiple publications, possibly even in top-tier journals, with Taylor as the prestigious first author on the papers (and her advisor as the final author).

In his absence, however, the last experiment (#6) did not work. Before this, Taylor has been able to successfully predict accurate rate constants over a wide range of temperatures using two different theories for her simulations. For this final test, however, neither set of simulations is correct, and Taylor cannot reproduce the same curves from before. Even with repeated attempts, there seems to be something wrong with the quantitative models, the apparatus, or both. Despite these challenges, her advisor cannot meet this week and tells Taylor by email to wrap everything up so she can defend "as soon as possible." Rather than delay the process and jeopardize her postdoc, Taylor chooses to just drop the negative experiment and focus on the other positive ones. Her advisor does not seem to mind, as he never mentions it in his comments on her draft.

A month later, Taylor defends and passes, without mentioning the last experiment. Her dissertation committee is floored with excitement over the implications of her findings, both theoretically and for possible industrial applications. They strongly encourage her to submit the first half of her dissertation to a mid-tier journal and the second half to a top-tier, high-impact journal. When Taylor begins her postdoc, her new Principle Investigator (PI) is also thrilled with her results. She allows Taylor to spend the first month finalizing and submitting her manuscripts, which receive stellar peer reviews and are quickly accepted and published online. Taylor's new PI is very proud of her, so she gives Taylor an exciting new project that also involves simulations but in a different area of chemical engineering. Taylor decides to leave the old project behind, figuring someone else will figure out what went wrong with her final experiment.

Discuss in your small groups:

1. **Has Taylor committed research misconduct?** Why or why not?
2. **Might anything here count as a "questionable research practice"?** If yes, what?
3. **Is there any behavior in the scenario that is ethically wrong?** Why or why not?

Case Study 2: Extreme Weather, Extreme Uncertainty
Chris ChoGlueck (ed. Alex Rinehart)

You just began your first job as a postdoctoral researcher at a well-known university with a leading expert in climate modeling. Earlier this year, you defended your dissertation on modeling extreme-weather events. Your supervisor is the PI on a project about the current mega drought and the extreme wildfires throughout the American Southwest. Your lab is currently exploring the relationship between climate variables and extreme wildfires over the past millennium, by first dating the frequency of large-scale fires throughout the region and then correlating them with the frequency of precipitation, temperature, vegetative cover, etc. This project involves extensive data collection and computer modeling over hundreds of years.

Before "getting into the real modelling," your PI tells you to send out to the lab some samples of wildfire data for basic analysis. While you can easily use tree-ring data to determine the severity and duration of droughts over the past thousand years, analyzing fires is a bit more challenging: Dating each event and determining its severity requires analysis of the organic carbon and black carbon released during combustion of plant tissue. Interference is common via leaching and biodegradation of the carbon. To correct for this, researchers have developed new methods for processing samples more systematically before the final analysis.

Your PI suggests you utilize the traditional method that she is very familiar with for forest-fire analysis. However, in your dissertation, you utilized a newer technique, which you favored for its increased precision and accuracy, even though the process takes twice as long to accomplish and costs twice as much as the older method. You have samples analyzed both ways.

Now, looking at the lab report, you find that you are not reproducing the expected results: Internally, each sample is reproducible to itself and compared to lab standards; however, the results of each method are inconsistent with some external data to different degrees. When comparing the results of the traditional method to the known wildfires over the past 100 years as recorded by the US government, only 75% of the events are replicated. With your favored newer technique, the results seem more accurate, reproducing the known events 90% of the time.

When you bring this up to your PI, she insists that "you must be doing something wrong." She is also concerned about the costs of your dating techniques, so you send more data into the lab for analysis with the older method. But, after another couple of weeks, you are even more convinced that your initial position is correct. You start to question your PI's judgment, who has not been at the bench for years and depends on students and postdocs for sampling & analysis. She keeps underplaying the need to correct the data and says you can fix the inconsistency later using a "fudge factor" to calibrate it against the known data. You are uncomfortable but entirely dependent on your PI for another two years, and she is correct that you are less experienced with traditional methods. You also don't want risk future employment problems, fearing that the discrepancy might be your fault.

Discuss the following in your small groups:

1. **What are the different possible actions** you could take to resolve this situation?
2. What are the **costs** and **benefits** of each?
3. **Which of the options is the best, ethically & scientifically?** Why?