Survey Questions

Below is a list of survey questions as presented to our participants

Consent

1. I have read and understood the participant information sheet linked above and have had the opportunity to ask questions about the survey. I agree to take part in this survey and agree for my data to be used for the purpose of this study. I understand that my participation is voluntary and I may withdraw (at any time) for any reason without my participation rights being affected.

    Yes

Recording & Storing your data

2. For each of the following types of work, how do you currently record it?

    Matrix

	On Paper	Electronically	A mix of both	N/A
Doing an experiment in the lab				
Doing an experiment outside of the lab				
Looking at literature				
Thinking about / planning your work				
Performing calculations to support your research				
Analysing your data				
Writing up your work				

3. How is your work organised / linked together **within a project**?

    Free text

4. How is your work organised / linked together **between projects**?

    Free text

Structural Representation

5. What does the term 'structure' mean to you in your research?

    Free text

6. When is it important to use digital representations of structure in your research?

    Free text

7. Which of the following structure representations do you use when communicating or undertaking your research?

    Multiple Selection

    - Formula / Composition
    - Compound Name
    - Structure Diagram
    - Computational Chemistry Formats

- Crystallographic formats (e.g. CIF)
- Chemistry Formats (e.g. MOL file, SMILES)
- Identifiers (e.g. InChI, CAS registry numbers)
- None of the above
- Other

Software & Collaboration

8. Do you make use of any digital research notebooks? If so, which ones?
   E.g. OneNote, Jupyter Notebooks, MBook, LabArchive, SciNote, RSpace
   Free text

9. Do you use software specifically for collaborating with colleagues / sharing research? If so, which software?
   Free text

10. What other software do you use in your research?
    Please list software names and include web-based or specialist / domain-based software if used.
    Free text

Sharing your data

11. Are you making your data available to others, if so how? (e.g. Via a repository or GitHub)
    Free text

12. Does it conform to FAIR standards?
    (Findable, Accessible, Interoperable, Reusable)
    Radio button
    - Yes
    - Partially
    - No
    - I'm not familiar with FAIR
    - N/A I don't share data

13. Are there any restrictions that you have encountered either whilst sharing or accessing data?
    Free text

Enabling your future research

14. Since the COVID-19 pandemic have you changed your research methods with respect to recording and sharing your work? If so, what aspects are digital that didn't used to be?
    Free text

15. Are any aspects now no longer digital that used to be?
    Free text

16. Do you think these changes will be permanent?
    Free text

17. Are there limitations or barriers in your current systems that prevent your research from reaching its full potential, if so what?
    Free text

18. Assuming a fully digital world, please select up to five features that would be important to your work
    Matrix

	1st – Most important	2nd	3rd	4th	5th	Lower than 5th / not important
Access to reference quality data						
Easily combining data from multiple sources						
Publishing data						
Repositories						
Availability of standards e.g. metadata, file formats, ontologies etc						
Platform for recording and managing data / information.						
Access to compute infrastructure / platforms for running code						
Exploiting AI / Machine Learning methods						
Bringing together experimental and simulation data						

19. If technology could do one thing to make your work easier, what would it be?
    Free text

About you and your research

20. What research area(s) do you work in?
    Free text
21. Please provide a description of the type of data that you work with
    Free text
22. With respect to your research, which of these roles do you undertake? (Please select all that apply)
    Multiple selection
    - Creating Data Management Plans
    - Generating new data
    - Obtaining existing data
    - Analysing data
    - Managing data
    - Curating data
    - Sharing & Publishing data
    - Other
23. Is there anything else relevant that you would like to tell us about this subject?

Free text
24. Would you be willing to be contacted to take part in a Focus Group as a follow up to this questionnaire? If so please put your name and email address in the box below.
Free text
25. Where are you based?
Radio button
- In the UK
- Outside the UK