## UNIVERSITY OF PLYMOUTH

**FACULTY OF SCIENCE AND ENGINEERING**

**Consent Form**

CONSENT TO PARICIPATE IN RESEARCH PROJECT / PRACTICAL STUDY

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Name of Principal Investigator

**Sophie Turner**

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Title of Research

**Molecular geometry prediction software feedback from scientists**

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Brief statement of purpose of work

I am a final year student of computer science at the University of Plymouth and I am creating a chemistry application for my dissertation project. I am looking for feedback and recommendations from chemists and other relevant scientists regarding the design of this application. These forms are anonymous but will be discussed in, and appended to, my dissertation report. Your name will **not** be included in this. You can request that your answers be deleted and not included in the project by emailing me at [sophie.turner@plymouth.ac.uk](mailto:sophie.turner@plymouth.ac.uk)

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The objectives of this research have been explained to me.

I understand that I am free to withdraw from the research at any stage, and ask for my data to be destroyed if I wish.

I understand that my anonymity is guaranteed, unless I expressly state otherwise.

I understand that the Principal Investigator of this work will have attempted, as far

as possible, to avoid any risks, and that safety and health risks will have been

separately assessed by appropriate authorities (e.g. under COSHH regulations)

Under these circumstances, I agree to participate in the research.

Name: ……………………………………….

Signature: .....................................…………….. Date: ……………………..

Molecular geometry prediction software feedback from scientists

1. Which science are you mostly involved in?
2. What is your role in this science (e.g. undergraduate, technician, etc)?
3. Please name all the software you have used for chemical structure/geometry modelling, e.g. GaussView, PubChem, Avogadro, etc. If you have never used software for this purpose, please skip to question 8.
4. Regarding the most recent time you used this software, please describe what you used the software for.
5. Why did you choose this software over others?
6. What do you consider to be the best things about this software?
7. What do you consider to be the worst things about this software?
8. In your opinion, what would be the most important features of software for predicting the geometric structure of a theoretical molecule? What would you want to be able to do, as a user of this software?

1. An evolutionary algorithm is a computer algorithm which can be used to find solutions to problems by following these steps:

* **Start with an initial estimate of a solution to a problem**, e.g. the positions of atoms in a molecule.
* **Alter variables which affect this solution**, e.g. the distance between the atoms.
* **Pass these variables to a function**, e.g. an energy calculation, **which returns an output – another possible solution**, e.g. the energy of the system.
* **Compare this solution to the previous solutions**.
* **Choose the best solution**, e.g. the lowest energy of the system.
* **Repeat these steps until reaching an optimal solution**, e.g. the bond lengths which create the lowest net force on each atom.

Algorithms like this can be used to predict geometric properties of molecules, such as bond lengths and bond angles. As a user of this software, do you think it would be useful to be able to view this process and adjust parts of the algorithm, such as which variables to change, or would you prefer it to be a ‘black box’ that worked behind the scenes and just showed you the output?

1. Was this questionnaire easy to understand and fill out? Is there anything that you think should be changed about it?
2. Is there anything else you would like to mention which could be useful for this project?

Thank you for your time. Please return your completed form to [sophie.turner@plymouth.ac.uk](mailto:sophie.turner@plymouth.ac.uk)