## 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 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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By participating in this usability test, you agree that:

* The objectives of this research have been explained to you.
* You understand that you are free to withdraw from the research at any stage, and ask for your data to be destroyed if you wish.
* You understand that your anonymity is guaranteed, unless you expressly state otherwise.
* You 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, you agree to participate in the research.

For each task, please comment on whether the program worked as expected and how easy it was to use. Please also mention any bugs you find.

Date: 25/1/21

**Task 1.** Please select up to eight atoms from any combination of H, C, O, N and/or Al. Ions and other elements are not yet supported by this program. You can select more than eight atoms if you wish to do so, but the algorithm may take some minutes to perform its calculations as the time taken rises exponentially with the size of the molecule.

Comments:

**It worked as expected.**

**Task 2**. View information about the structures and potential energy surfaces.

Comments:

**Very good UI and nice graphs. Don’t understand them though.**

**Task 3**. Create another system of atoms.

Comments:

**I chose N N O O and it said it was not a valid molecule. Didn’t work.**

**Task 4.** View information about the structures and potential energy surfaces.

Comments:

Did you find this form comprehensive and easy to complete?

**Yes.**

Additional comments and suggestions:

Perhaps you could let the user choose how long it takes, how many iterations etc.

Thank you for your time.