## 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:

***10/02/2021***

**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:

Program worked? Y

Easy to use? Y

I used HCN as the example. HCN is a linear molecule with a triple bond between C and N. The results were unexpected; the structure with the H atom closer to both C and N was lower in energy than the more linear structure with 180 degree bond angles between H, C and N. The program appears to only be able to anticipate singly bonded molecules.

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

Comments:

Program worked? Y

Easy to use? Y

Structure information is excellent. It is easy to see the molecules in 3D. It might be nice to be able to rotate the structure diagrams to see more detail about the arrangement of atoms. The PES is good. Can’t understand the ‘All positions tested’ part. The colours all overlap.

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

Comments:

This time I used CH2N. The structures were clear, and the lowest energy structure was again unexpected.

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

Comments:

It’s still difficult to interpret the positions tested and the 3D plot is difficult to read when there are more atoms.

Did you find this form comprehensive and easy to complete?

Yes

Additional comments and suggestions:

You could add a separate yes/no section to the feedback form to make it easier to interpret whether the form was user friendly.

Thank you for your time.