Molecular geometry prediction software feedback from scientists

1. Which science are you mostly involved in?

*Chemistry*

1. What is your role in this science (e.g. undergraduate, technician, etc)?

*BSc (Hons) Chemistry*

1. Please name all the software you have used for chemical structure/geometry modelling, e.g. GaussView, PubChem, Avogadro.cc, etc. If you have never used software for this purpose, please skip to question 8.

Chemdraw, GaussView

1. Regarding the most recent time you used this software, please describe in more detail what you used the software for.

GaussView – Approximate energies of molecular orbitals

Chemdraw – Model skeletal formula in organic chemistry and interactions between molecules

1. Why did you choose this software over others?

Chemdraw – free licence

GaussView – free licence

1. What do you consider to be the best things about this software?

Chemdraw – User-friendly, made by chemists so valencies and structures are sensible.

GaussView – Fast, user-friendly, 3D representation of orbitals on structure given.

1. What do you consider to be the worst things about this software?

Chemdraw – Sometimes incorrectly corrects valencies when working with unusual structures so it can be difficult when working with novel systems

GaussView – Only allows energies to be computed for single systems. Small structural size limits to reduce computational expense.

1. 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?

* Easy to use
* Designed by chemists
* 360 degree view of finished molecule
* Able to model interactions between different systems of molecules

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 or function**, 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?

*View and adjust, with option to make output simpler when required*

1. Was this questionnaire easy to understand and fill out? Is there anything that you think should be changed about it?

*Good questionnaire.*

1. Is there anything else you would like to mention which could be useful for this project?

*An option to analyse the interactions of structures in different solvents would be good.*

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