Participant Information

Thank you for choosing to participate in this Solubility panel.

We are examining the hypothesis that human experts are as good as computation in predicting aqueous solubility of organic molecules.

You will be asked for information about your level of formal education and your current (or most recent) field of employment, work or study.

You will then be asked to predict the aqueous solubility (in logarithmic units referred to moles per litre) of 50 druglike organic molecules.

We will endeavour to use compounds whose solubilities are experimentally known, but are not so common or significant as to be widely disseminated. However, we may throw in some better known compounds to test how this affects the results. If you believe that you know the solubility of a compound accurately, please enter this value as your prediction anyhow.

Please do not use reference books, papers or the internet to look up solubility values while taking the survey. You can choose not to make an estimate for a compound if you so wish. You may withdraw from the survey at any time.

After data collection, the raw data will be analysed and results entered into a spreadsheet. Since the data are anonymous, we do not anticipate any significant risk to the respondents’ anonymity or security. Data will be securely stored on these computers indefinitely. In the event of publication, anonymous data from the study will made available on the University’s Research Repository, Pure, as data supporting the relevant paper. Data will be processed using computers within the University.

At the end of the survey you will be shown a page of debriefing information.

Consent Form
This research has been scrutinised and been granted Ethical Approval through the University of St Andrews ethical approval process.

All your responses to this survey will be anonymous. Data will be handled securely and you will not be identifiable by your responses.

Once again you may choose to leave any question blank and may leave the survey at any point.

By continuing you are consenting for your responses to be used in our research.

Instructions

You will be shown 25 drug-like molecules.

Your task is to predict the solubility, in logarithmic units of mol/L, of each molecule.

To help you we have compiled a set of training data.

The training data consists of 75 molecules and their solubilities.

Click here to launch the training data in a new tab.

Qualification and Job
What is the highest level of qualification you have gained?

- A-Level/Scottish Highers (School leavers level)
- First undergraduate degree (e.g. BSc/MChem)
- PhD/Doctorate
- Other

What is your current (or most recent) occupation?

- Undergraduate Student
- Postgraduate Student
- Research academic
- Pharmaceutical industry
- Other

**solubility question 1**

![Chemical structure of 4-aminosalicylic acid](attachment:image.png)

4-aminosalicylic acid

Refer to the [training data](https://standrews.eu.qualtrics.com/ControlPanel/...). What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?
solubility question 2

Refer to the training data.
What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

antipyrene

solubility question 3

Refer to the training data.
What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

4-aminobenzoic acid

solubility question 4
Refer to the training data.
What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

corticosterone

solubility question 5
Refer to the training data.
What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

**solubility question 6**

![Dapsone](image)

Refer to the training data.
What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

**solubility question 7**

![Primidone](image)

Refer to the training data.
What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

**solubility question 8**

Refer to the training data.
What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

**solubility question 9**

alclofenac
Refer to the training data. What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

**solubility question 10**

![Molecule 1](image1)

5-fluorouracil

Refer to the training data. What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

**solubility question 11**

![Molecule 2](image2)

griseofulvin

Refer to the training data. What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?
solubility question 12

[Chemical structure of fluometuron]

fluometuron

Refer to the training data. What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

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solubility question 13

[Chemical structure of fluconazole]

fluconazole

Refer to the training data. What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?
solubility question 14

Refer to the training data. What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

solubility question 15

Refer to the training data. What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?
Refer to the training data.
What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

**solubility question 16**

![norethisterone](image)
norethisterone

Refer to the training data.
What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

**solubility question 17**

![nicotinic acid](image)
nicotinic acid

Refer to the training data.
What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?
solubility question 18

Refer to the training data.
What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

perphenazine

solubility question 19

Refer to the training data.
What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

pteridine
solubility question 20

Refer to the training data.
What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

![salicylamide](image)

salicylamide

solubility question 21

Refer to the training data.
What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

![sulfanilamide](image)
sulfanilamide
solubility question 22

![Gliclazide structure](image)

**gliclazide**

Refer to the [training data](https://standrews.eu.qualtrics.com/ControlPanel/...).

What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

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solubility question 23

![Trihexyphenidyl structure](image)

**trihexyphenidyl**

Refer to the [training data](https://standrews.eu.qualtrics.com/ControlPanel/...).

What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?
solubility question 24

Refer to the training data.
What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

triphenylene

solubility question 25

Refer to the training data.
What is the aqueous solubility, in logarithmic units of mol/L, of this molecule?

mifepristone
Debriefing Information

Thank you for taking part in our Solubility Panel exercise. Your help is greatly appreciated.

We are testing the hypothesis that human experts are as good as computation in predicting aqueous solubility of organic molecules. Your responses will be collated and compared to computational methods. We will be using a chemoinformatics-based a machine learning approach to computationally predict solubility. The performance of the participants and computations will be compared and statistically analysed.

We hope to publish the results, but emphasise that no Panel member will be individually identifiable. We will be happy to answer any queries about this project and provide more information (jbom@st-andrews.ac.uk; 01334 467259).