

Welcome screen

ProtoPRED

Contact form Log in ABOUT EN ES FR IT

ProtoICH ProtoREACH ProtoPHYSICHEM ProtoTOX ProtoECO ProtoADME TRY OUR DEMO

ProtoPRED is a computational platform allowing the easy, fast and user-friendly prediction of different properties of chemical compounds, including regulatory endpoints and others, such as:

- Physico-chemical properties
- Pharmacokinetics properties (ADME)
- Human toxicity
- Ecotoxicity

ProtoPRED uses proprietary QSAR (Quantitative Structure-Activity Relationships) models. These models are widely applied in different sectors, such as cosmetics, pharmaceuticals and chemicals, to predict a broad-spectrum of properties of industrial and regulatory interest. Our wide library of proprietary models are grouped in different modules, based on the type of property. User can select the model(s) that best match their requirements.

ProtoICH
Mutagenicity
MORE INFO ACCESS

ProtoREACH
REACH-related endpoints
MORE INFO ACCESS

ProtoADME
ADME endpoints
MORE INFO ACCESS

ProtoPHYSICHEM
Physicochemical endpoints
MORE INFO ACCESS

ProtoTOX
Toxicological endpoints
MORE INFO ACCESS

ProtoECO
Ecotoxicological endpoints
MORE INFO ACCESS

- 1 Switch between ProtoPRED modules
- 2 Contact form
- 3 Log in/log out
- 4 About section (manuals, contact information and more)
- 5 Switch language
- 6 Access ProtoICH (as an example)

Log in screen

ProtoPRED

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LOGIN DATA

Username:

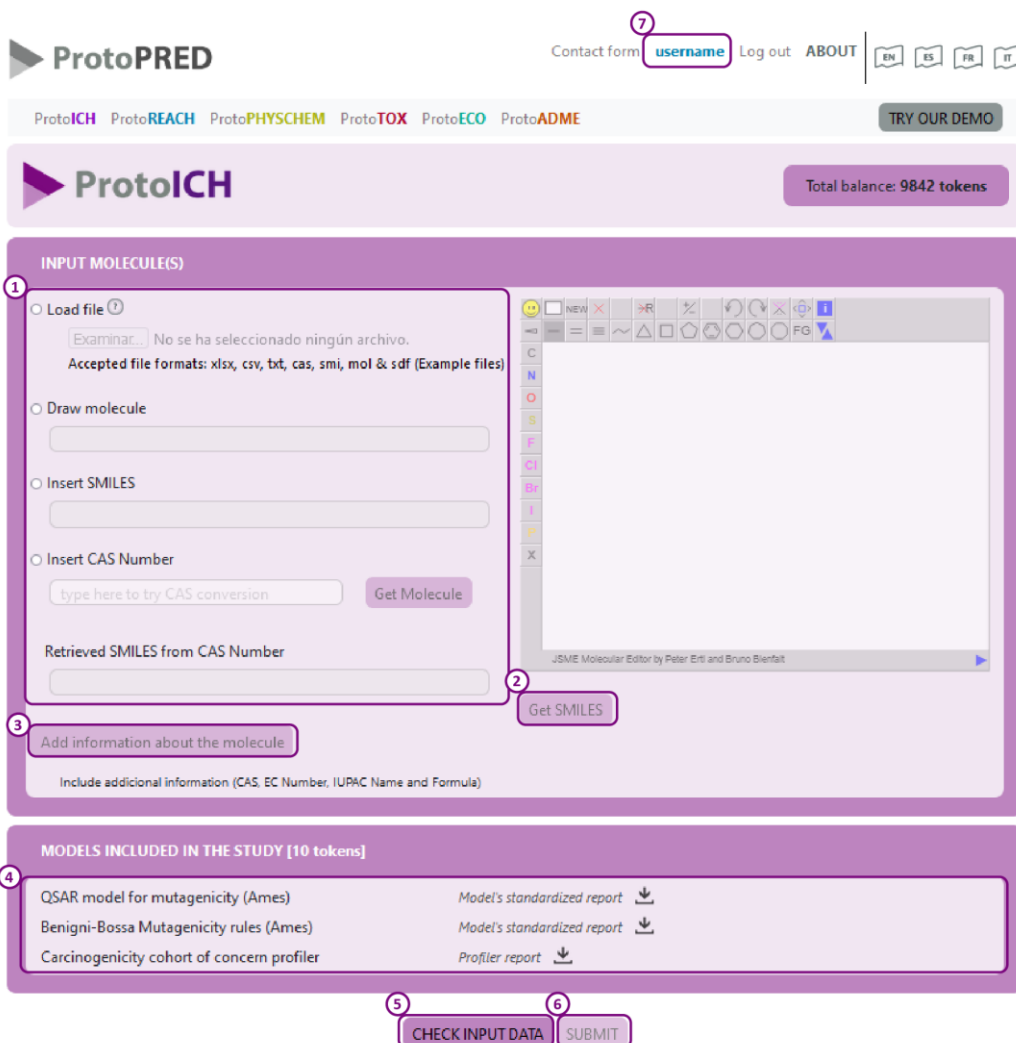
Password:

Log in

Do you want to request information or register? Please [Contact us](#)

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Input data screen (ProtoICH)



The screenshot shows the ProtoICH web interface. At the top, there is a navigation bar with the ProtoPRED logo, a contact form with a 'username' field, and links for 'Log out' and 'ABOUT'. Language selection icons for EN, ES, FR, and IT are also present. Below this is a secondary navigation bar with links for ProtoICH, ProtoREACH, ProtoPHYSICHEM, ProtoTOX, ProtoECO, and ProtoADME, along with a 'TRY OUR DEMO' button. The main header for ProtoICH shows a 'Total balance: 9842 tokens'.

The main content area is titled 'INPUT MOLECULE(S)' and contains several input options:

- 1** **Load file**: A file selection button with a dropdown arrow. Below it, a message states 'No se ha seleccionado ningún archivo.' and lists accepted file formats: 'xlsx, csv, txt, cas, smi, mol & sdf (Example files)'.
- Draw molecule**: A simple drawing interface with a toolbar and a canvas.
- Insert SMILES**: A text input field for entering SMILES strings.
- Insert CAS Number**: A text input field for entering CAS numbers, with a 'Get Molecule' button next to it.
- Retrieved SMILES from CAS Number**: A text input field for displaying the SMILES string retrieved from a CAS number.
- 2** **Get SMILES**: A button located below the retrieved SMILES field.

Below the input options is a section for adding additional information:

- 3** **Add information about the molecule**: A text input field with a label 'Include additional information (CAS, EC Number, IUPAC Name and Formula)'.

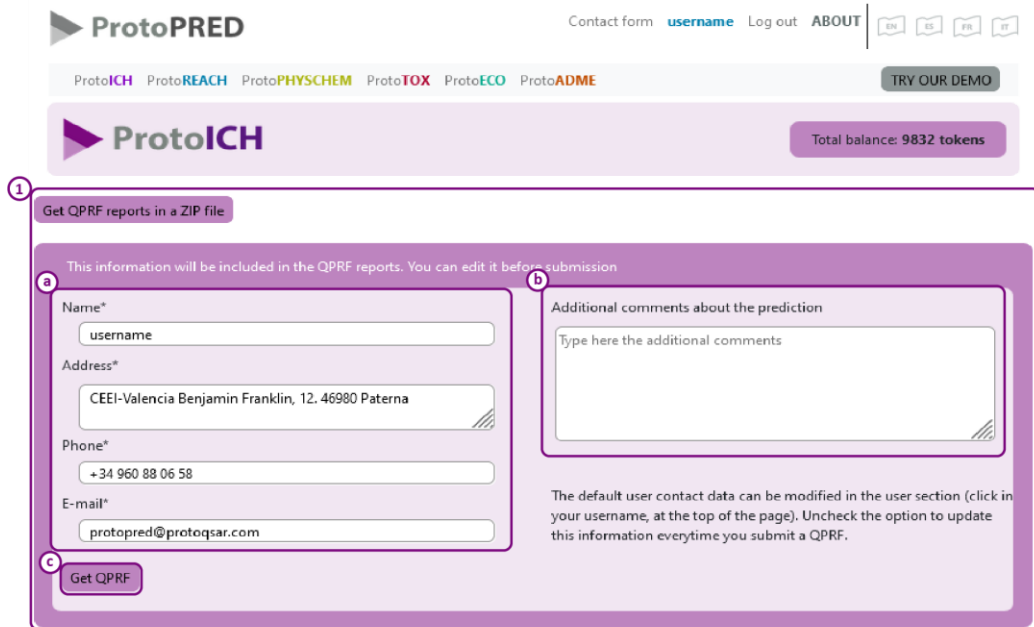
The bottom section is titled 'MODELS INCLUDED IN THE STUDY [10 tokens]' and contains a table of models:

Model Name	Report Type	Action
QSAR model for mutagenicity (Ames)	Model's standardized report	Download icon
Benigni-Bossa Mutagenicity rules (Ames)	Model's standardized report	Download icon
Carcinogenicity cohort of concern profiler	Profiler report	Download icon

At the bottom of the screen, there are two buttons: **5** **CHECK INPUT DATA** and **6** **SUBMIT**.

- 1** Insert molecule(s). Choose one of the following options:
 - Load file
 - Draw molecule
 - Insert SMILES
 - Insert CAS
- 2** Edit SMILES/retrieve SMILES from drawing
- 3** Include additional information about the molecule:
 - EC number
 - IUPAC name
 - Structural formula
- 4** Select endpoints
- 5** Structure check. Verification of structure(s) consistency is performed
- 6** Run prediction
- 7** Access user profile

Results screen (ProtoICH)



1 Get prediction reports in PDF

- a Change user information (optional)
- b Add additional comments about the prediction (optional)
- c Get reports

2 Get results table in .xlsx format.

2 Get results table in an XLSX file

Statistical (QSAR) Mutagenicity (Ames test)

ID	Chemical name	EC number	Structural formula	CAS	SMILES	Experimental value*	Predicted value	Reliability	Applicability domain**
0_CCCCC	-	-	-	-	CCCCC	Non-mutagenic	Non-mutagenic	92.44 %	Inside (Tanimoto)

* Experimental values are provided when available.

** The AD is determined by different methods. The most suitable method is indicated.

Benigni-Bossa Mutagenicity rules (Ames)

ID	Chemical name	EC number	Structural formula	CAS	SMILES	ALERTS SUMMA
0_CCCCC	-	-	-	-	CCCCC	NO ALERTS DETECTED

Carcinogenicity cohort of concern profiler

ID	Chemical name	EC number	Structural formula	CAS	SMILES	CoC SUMMARY ALE
0_CCCCC	-	-	-	-	CCCCC	NO ALERTS DETECTED