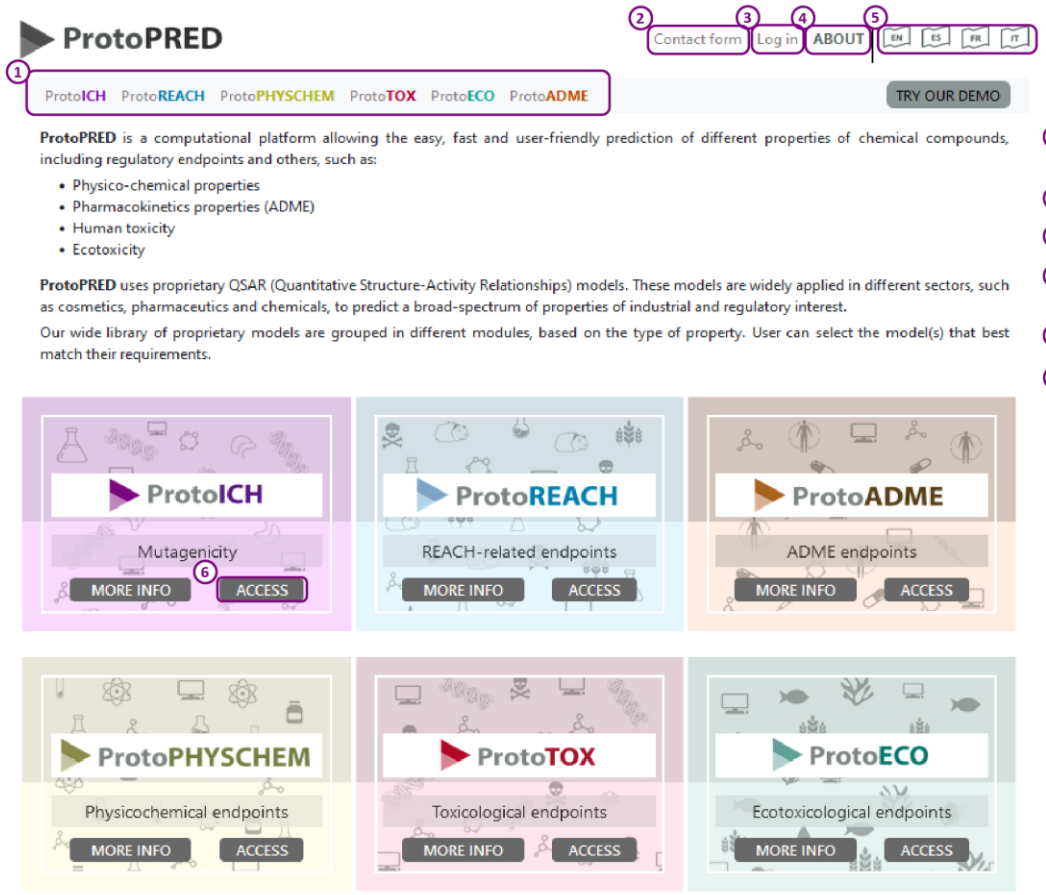
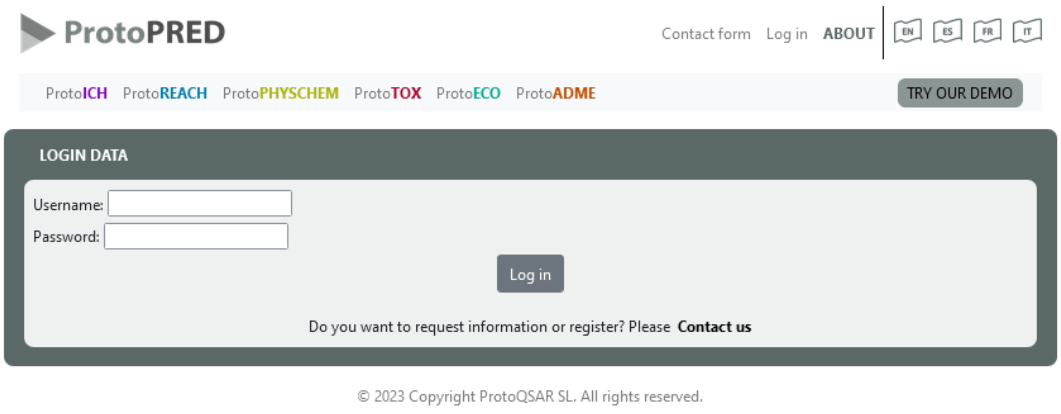
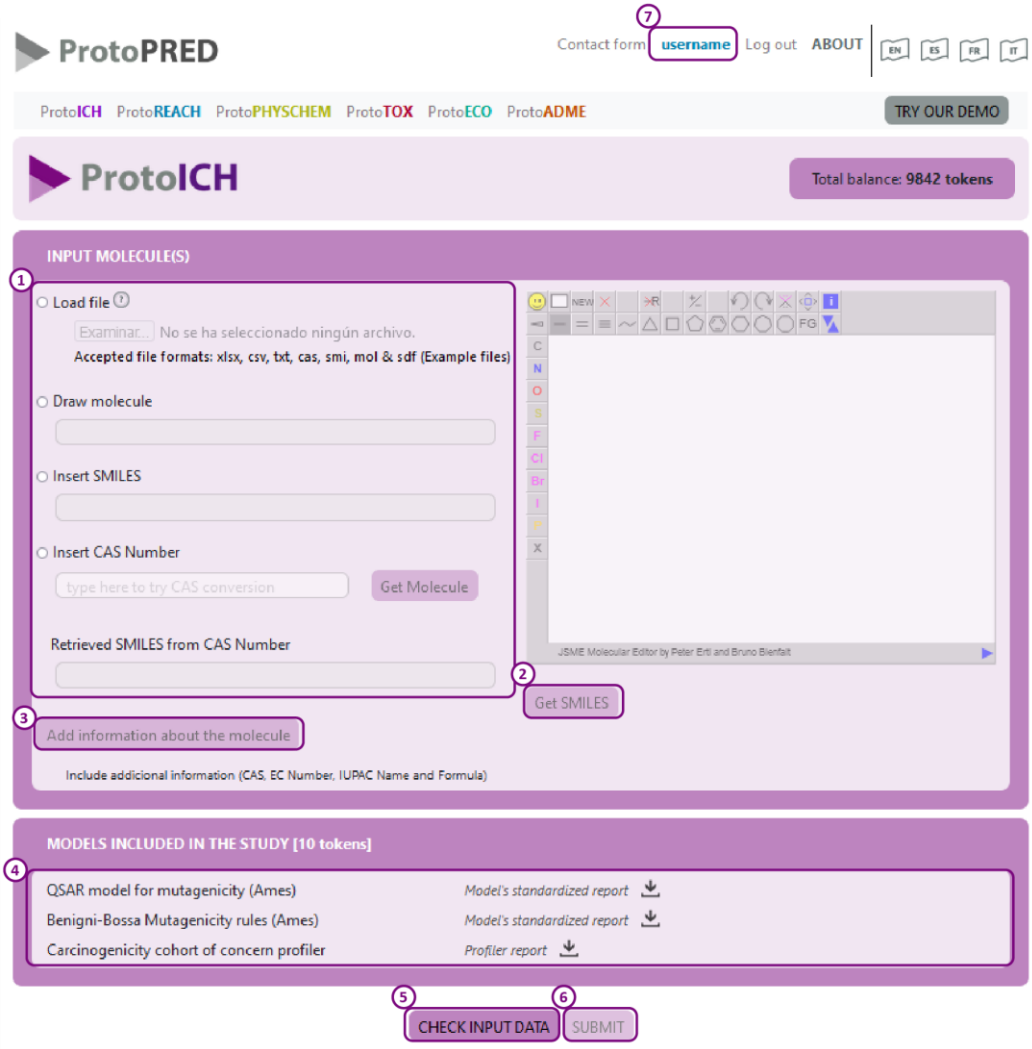
Welcome screen



Log in screen

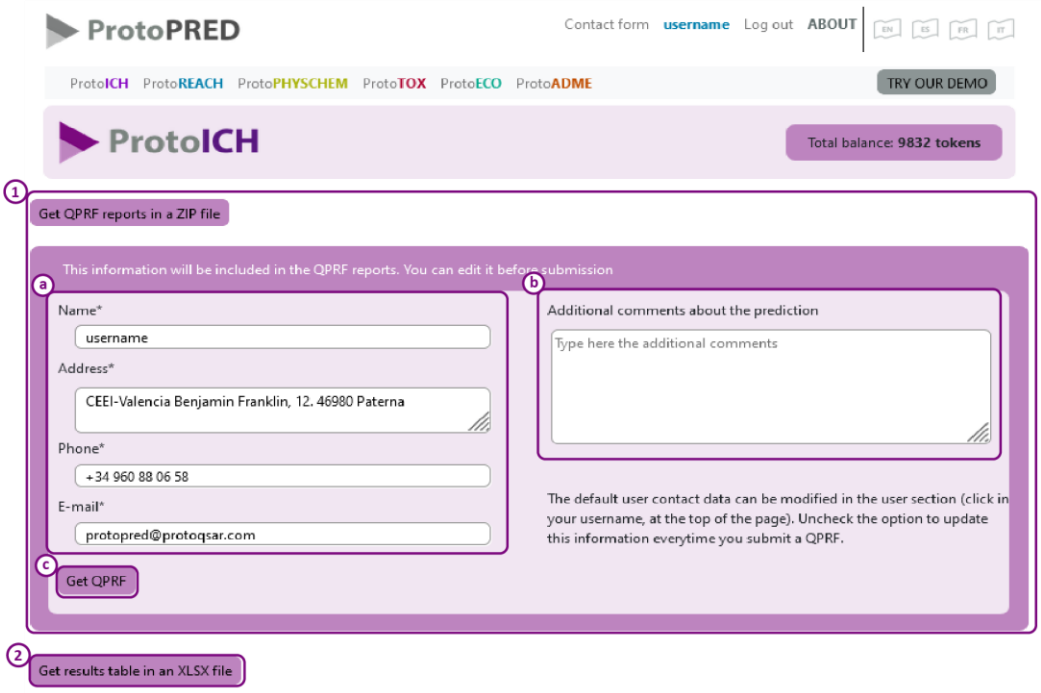


Input data screen (ProtoICH)



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 addicional 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.

Statistical (QSAR) Mutagenicity (Ames test)

ID	Chemical name	EC number	Structural formula	CAS	SMILES	Experimental value*	Predicted value	Reliability	Applicabilit 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	