pkCSM: predicting small-molecule pharmacokinetic properties using graph-based signatures

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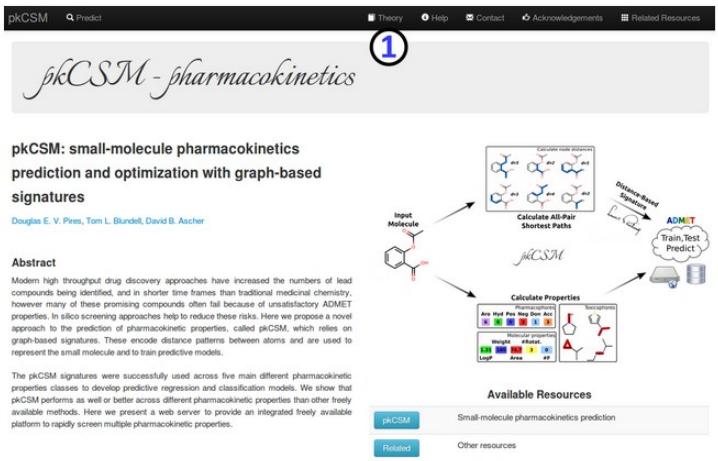
Main page



About pkCSM

pkCSM is a machine-learning platform to predict small-molecule pharmacokinetic properties, which relies on distance/pharmacophore patterns encoded as graph-based signatures. The platform is composed of 22 regression and classification models, trained and tested on different experimental data sets encompassing a diverse and complementary set of ADMET descriptors as follows:

- **Absorption**: Caco-2 permeability, water solubility, intestinal absorption (human), P-glycoprotein substrate and inhibitor.
- **Distribution**: Volume of distribution (human), fraction unbound (human) BBB and CNS permeability
- **Metabolism**: Cytochrome P450 inhibitor and substrate
- **Excretion**: Renal OCT2 substrate
- **Toxicity**: Rat LD50, AMES toxicity, *T.Pyriformis* toxicity and Minnow toxicity

More information about the predictive models and **how to interpret the pkCSM predicitons** can be accessed via the Theory menu (1).

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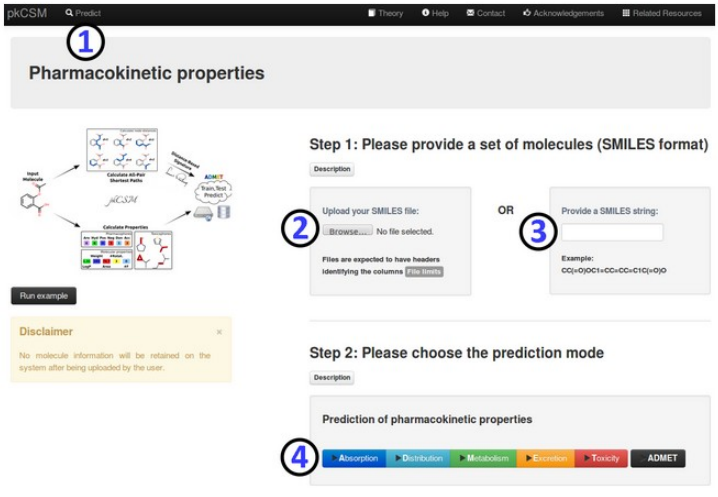
Submission page



How to run a prediction

To run a prediction:

- Click on "Prediction" **(1)** to open the submission page.
- Provide either an input file with a list of molecules (2) in SMILES format (up to a maximum of 1000 molecules) or supply a single SMILES string (3). Users are advised to use Canonical SMILES. Syntax non-compliant molecules will be ignored.
- The next step is to choose the prediction mode (4). Users can choose between the main **ADMET** property classes (**A**bsorption, **D**istribution, **M**etabolism, **E**xcretion and **T**oxicity) by clicking on its corresponding button or run a systematic evaluation of all predictive models.

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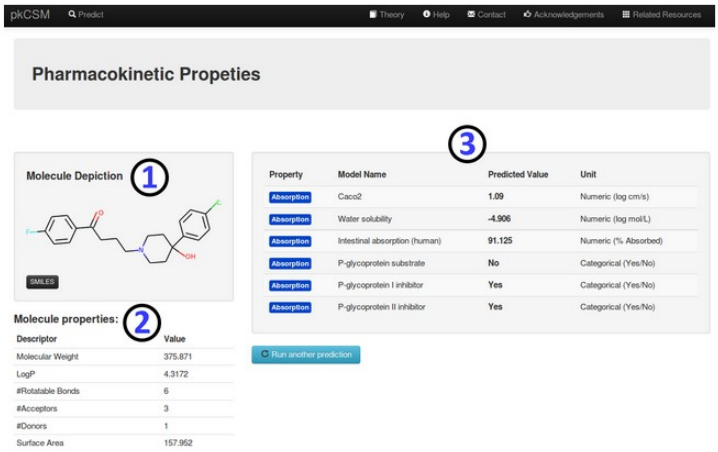
Results page



Results

For a **single molecule** prediction, your results can be displayed as follows:

- A **depiction** of the uploaded molecule will be shown in (1). Make sure the depiction is what you are expecting for your molecule.
- A list of **molecule properties** will be calculated and shown in (2).
- The prediction will be displayed in a tabular format as presented in (3). The information shown include the **ADMET property** being predicted, **model name**, the actual **predicted value** and whether the prediction is **numeric** (for regression models, including the unit of the predicted value) or **categoric** (for classification models).

Results for **multiple molecules** will be shown in a tabular format, whithout molecule depiction, which can be downloaded as a CSV file.

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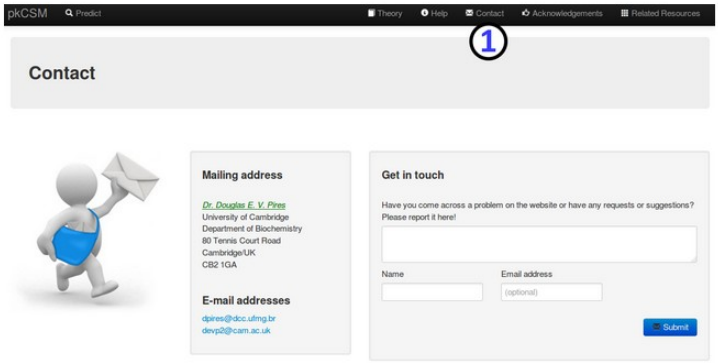
Contact page



Getting in touch

In case you experience any trouble using pkCSM or have any suggestions or comments, please do not hesitate in contacting us (1) either via e-mail or through the online form.