pdCSM-GPCR: predicting potent GPCR ligands with graph-based signatures

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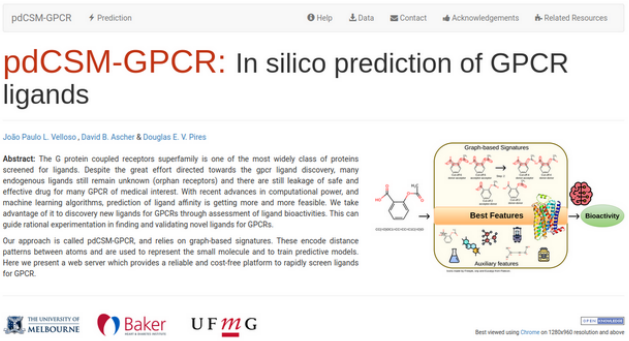
Help - How to use pdCSM-GPCR

Main page



About pdCSM-GPCR

pdCSM-GPCR is a machine-learning platform to predict GPCR ligands, which relies on distance/pharmacophore patterns encoded as graph-based and auxiliary signatures. The platform is composed of 36 regression models, trained and tested on different experimental data sets encompassing a diverse and complementary set of GPCRs as follows:

- **Class A**: P08173, P08908, P08912, P0DMS8, P20309, P21452, P21917, P24530, P28335, P29275, P30542, P30968, P34995, P35346, P35348, P35372, P46663, P47900, P48039, P50406, P51677, Q8TDS4, Q8TDU6, Q96LB2, Q99500, Q99705, Q9H228, Q9HC97, Q9Y5N1, Q9Y5Y4;
- **Class B1**: P47871, Q16602;
- **Class C**: P41180, Q14416, Q14833;
- **Class F**: Q99835.

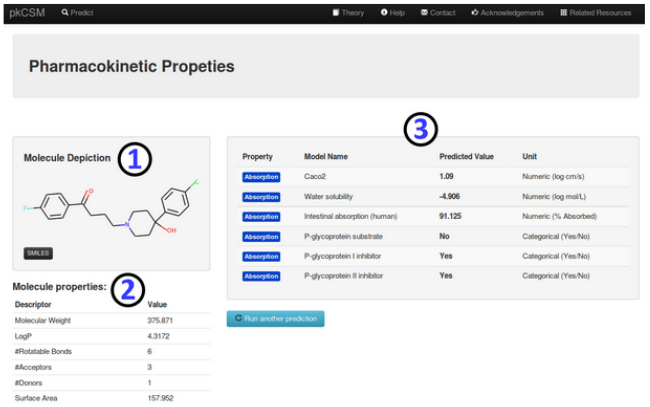
Submission page

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 100 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 type of prediction **(4)**. Users can choose between running **All** receptors at once or running class **A**, class **B1**, class **C** and class **F** receptors separately, by clicking on its corresponding button..

Results page



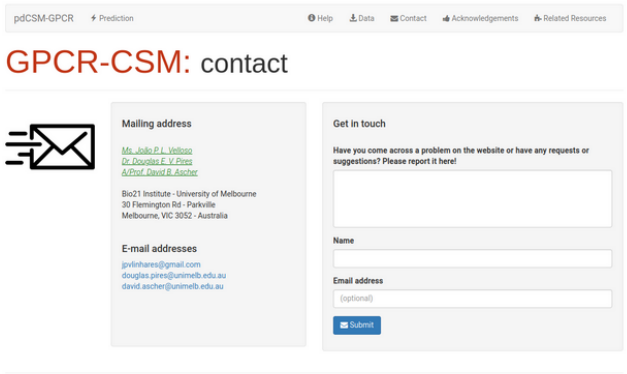
Results

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 is the **Bioactivity** being predicted and the actual **predicted value** in µMolar.

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

Contact page



Getting in touch

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