

# Interface overview

The screenshot displays the RavensAI ChemX interface for a project titled "BACE inhibition". The interface is divided into several sections:

- Header:** Includes the RavensAI ChemX logo, a user profile icon (D), a notification bell, and the username "admin".
- Left Sidebar (MENU):** Contains navigation options: Home, Modelling Projects, Standard Models, My Models, Screening Libraries, User Profile (B), Manuals and Tutorials, and Contact Support.
- Project Overview (C):** Shows tabs for Details, Molecules, Target Parameters, Models, and Explainability. Below the tabs is a table of molecules with columns for 2D Structure, Molecule Id, Warnings, and Smiles. The table lists 10 molecules, with the first one having a warning icon (yellow triangle).
- Right Panel (E):** A "WORKFLOW" section with five mandatory steps: 1. Check Molecules, 2. Check Target Data, 3. Featureize and Model Data, 4. Explain Model, and 5. Save Favorite Model.
- Bottom Right Panel (F):** An "ADDITIONAL ACTIONS" section with options: Reassign Parameter Type, Transform Data, Generate 3D structures, Detect Outliers, Remove Favorite Model, and Delete Project.

2D Structure	Molecule Id	Warnings	Smiles
	id: 2872976		<chem>NC1=NC@@(c2ccccc2c3ccccc3F)c2c2ccc3c(c2)OC(F)O3)C2=NCCCN12</chem>
	id: 2873000	▲	<chem>CC(=O)NC(Cc1cc(F)cc(F)c1)C(O)CNC1(c2ccccc(C)C)c2)CCCN(C(=O)O)Cc2ccccc2)C1</chem>
	id: 2872795	▲	<chem>CCCC1CNC(C(O)C(Cc2cc(F)cc(F)c2)NC(=O)C(O)N2CC(C)C(C)C2=O)C1</chem>
	id: 2872380	▲	<chem>CC(=O)NC(Cc1cc(F)cc(F)c1)C(O)CNC1(c2ccccc(C)C)c2)CCNC(=O)C1</chem>
	id: 2872811	▲	<chem>CCNc1cc(C(=O)NC(Cc2ccccc2)C(O)CNC2CC(C)C2)cc2e1CCCC(=O)(=O)N2C</chem>
	id: 2872500	▲	<chem>CC(C)C(O)c1cc(C2(c3ccccc34cnc4c3)N=C(N)N(C)C2=O)en1</chem>
	id: 2872847	▲	<chem>CN1C(=O)C(c2ccccc2c3ccccc3c2)c2ccc3c(c2)OC3)N=C1N</chem>
	id: 2872793	▲	<chem>CC(=O)NC(Cc1cc(F)cc(F)c1)C(O)CNC1(c2cc(C)C(O)C)c2)CC(C)C1</chem>
	id: 2872375	▲	<chem>Cc1cc2cc(n1)OCCCCOe1cccc(e1)C(C)C(O)CNC1(c3ccccc(C)C)c3)CC1)NC2=O</chem>
	id: 2871987		<chem>CN1C(=O)C@@(C@H)(c2ccccc2)c2ccccc2c3cc(F)ccc3)C2)N=C1N</chem>

**A** Navigate between modelling projects, completed models, and screening libraries.

**B** Access your User Profile, the Documentation and tutorials, or contact support.

**C** Use the tabs to switch between viewing project details, molecules, target data, models, and explanations. Project details include the molecule upload log.

**D** See ongoing tasks by clicking the hour glass, completed tasks by clicking the bell, and log-out by clicking your user name. It is possible to see the status of an ongoing task and kill it from within the hour glass panel. You can click on completed tasks (...) to go to their results.

**E** Here you will find the 5 mandatory steps for successful modelling.

**F** Additional actions that may be needed during modelling.