

Interface overview

The screenshot displays the RavensAI ChemX web interface. The top navigation bar includes the logo, a user profile icon (D), and an 'admin' link. A left sidebar (A) contains a 'MENU' with links to Home, Modelling Projects, Standard Models, My Models, and Screening Libraries. Below this is a 'B' section with links to User Profile, Manuals and Tutorials, and Contact Support. The main content area (C) is titled 'BACE inhibition' and features tabs for Details, Molecules, Target Parameters, Models, and Explainability. The 'Molecules' tab is active, showing 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. A search bar and 'Apply to All columns' dropdown are at the top right of the table. On the far right, a 'WORKFLOW' panel (E) lists five steps: Check Molecules, Check Target Data, Featureize and Model Data, Explain Model, and Save Favorite Model. Below this is an 'ADDITIONAL ACTIONS' panel (F) with options like Reassign Parameter Type, Transform Data, Generate 3D structures, Detect Outliers, Remove Favorite Model, and Delete Project. The bottom of the interface shows pagination information: Page Size: 10, 1 to 10 of 1,511, and Page 1 of 152.

2D Structure	Molecule Id	Warnings	Smiles
	id: 2872976		<chem>NC1=N[C@@H](c2ccccc2c3ccccc3F)c2(c2cc3c(c2)OC(F)F)O3)C2=NCCCN12</chem>
	id: 2873000	⚠	<chem>CC(=O)NC(Cc1cc(F)cc(F)c1)C(O)CNC1(c2ccccc2)C(C)C2)CCCN(C(=O)O)Cc2ccccc2)C1</chem>
	id: 2872795	⚠	<chem>CCCCC1CNC(C(O)C(Cc2cc(F)cc(F)c2)NC(=O)C(O)C2CC(C(C)C)C2=O)C1</chem>
	id: 2872380	⚠	<chem>CC(=O)NC(Cc1cc(F)cc(F)c1)C(O)CNC1(c2ccccc2)C(C)C2)CCNC(=O)C1</chem>
	id: 2872811	⚠	<chem>CCNe1cc(C(=O)NC(Cc2ccccc2)C(O)CNC2CC(C)C2)cc2c1CCCC(=O)C(=O)N2C</chem>
	id: 2872500	⚠	<chem>CC(C)COn1cc(C2(c3ccccc3c4cccc4c3)N=C(N)C(C)C2=O)cn1</chem>
	id: 2872847	⚠	<chem>ON1C(=O)C(c2ccccc2c3ccccc3c2)c2cc3c(c2)OC3)N=C1N</chem>
	id: 2872793	⚠	<chem>CC(=O)NC(Cc1cc(F)cc(F)c1)C(O)CNC1(c2cc(C(C)C)C2)CCCCC1</chem>
	id: 2872375	⚠	<chem>Cc1cc2cc(n1)OCCCCOe1cccc(e1)CC(C(O)CNC1(c3ccccc3)CC1)NC2=O</chem>
	id: 2871987		<chem>CN1C(=O)C[C@@H](c2ccccc2)c2ccccc2c3cc(F)ccc3F)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.