

RavensAI ChemX
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admin

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MENU

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C

Details

Molecules

Target Parameters

Models

Explainability

2D Structure	Molecule Id	Warnings	Smiles
	id: 2872976		<chem>NC1=NC@@@([c2ccccc(c3ccnc3F)c2](c2ccc3C(=O)OC(F)(F)O3)C2=NCCCN12</chem>
	id: 2873000	▲	<chem>CC(=O)NC(Cc1cc(F)cc(F)c1)C(O)CNC1(c2cccc(C(C)(C)C)CCN(C(C)=O)Oc2ccc2)C1</chem>
	id: 2872795	▲	<chem>CCCCC1CNC(C(O)C(Cc2cc(F)cc(F)c2)NC(=O)C(C)N2CCC(C(C)(C)Cz=O)C1</chem>
	id: 2872380	▲	<chem>CC(=O)NC(Cc1cc(F)cc(F)c1)C(O)CNC1(c2cccc(C(C)(C)C)CCN(C(C)=O)C1</chem>
	id: 2872811	▲	<chem>CCNc1cc(C(=O)NC(Cc2ccccc2)C(O)CNC2CCOC2Cc2c1CCCC(=O)N=O)N2C</chem>
	id: 2872500	▲	<chem>CC(C)Cn1cc(Cc2ccccc(c4cncc4)c3)N=C(N)N(C)C2=O)n1</chem>
	id: 2872847	▲	<chem>CN1C(O)C(c2ccccc(c3ccnc3)c2)(c2ccc3c(c2)OC(O)N=C1N</chem>
	id: 2872793	▲	<chem>CC(=O)NC(Cc1cc(F)cc(F)c1)C(O)CNC1(c2cc(C(C)=O)cc(C(C)(C)C)c2)CCCC1</chem>
	id: 2872375	▲	<chem>Cc1cc2cc(n1)OCCCCOc1cccc(c1)CC(C(O)CNC1(c3ccccc(C(C)(C)C)JC1)NC2=O</chem>
	id: 2871987		<chem>CN1C(O)C@@([c2ccnc2](c2ccccc(c3cc(F)cc3F)c2)N=C1N</chem>

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WORKFLOW

- 1 Check Molecules
- 2 Check Target Data
- 3 Featureize and Model Data
- 4 Explain model
- 5 Save Favorite Model

F

ADDITIONAL ACTIONS

- ↻ Reassign Parameter Type
- 🔗 Transform Data
- 🧬 Generate 3D structures
- ⚠️ Detect Outliers
- ❤️ Remove Favorite Model
- 🗑️ Delete Project

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

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.

F Additional actions that may be needed during modelling.