

# Manual

## ***in-mac* : Machine Generated Bioactivity Platform for Designing Analogs**

(A Bioassay Guided Tool for Potential Therapeutic Molecules)

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## **INTRODUCTION:**

Just as we test small molecules in the lab—through in-vitro and in-vivo experiments to study their bioactivity—we can now also evaluate them digitally using a new approach we call *in-mac* (short for “in-machine”). This platform allows us to predict the bioactivity of small molecules directly from their structure, without the need for physical experiments.

The *in-mac* system creates a simulated bioassay environment using real experimental data. Users can choose a biological target or cell line from a simple drop-down menu. Based on that selection, the platform calculates the molecule’s bioactivity—referred to as the *in-mac value*—using three key inputs:

1. The query molecule
2. A reference or control molecule
3. The machine-generated assay environment

In this way, *in-mac* acts as a virtual, bioassay-guided tool to help researchers design functional analogues and explore the potential of small molecules more efficiently.

The *in-mac* platform provides a way to digitally represent the bioactivity of small molecules based solely on their structure. Rather than simulating physical lab experiments, *in-mac* generates a machine-derived bioactivity value—known as the *in-mac value*—within a digitally constructed bioassay environment.

This environment is built using empirical data, and users can select a specific biological target or cell line from a drop-down menu. The *in-mac value* is then calculated based on three key components:

1. The structure of the query molecule
2. A chosen reference or control molecule
3. The selected digital bioassay environment

It's important to note that the *in-mac value* is **not** equivalent to in-vitro or in-vivo measurements. Instead, it should be interpreted in the context of the reference/control molecule within the same machine-generated assay environment. This makes *in-mac* a useful tool for guiding the design and evaluation of functional analogues (**devoid of any chemical series**) in a consistent, data-driven way.

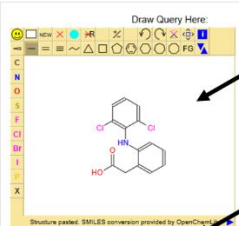
**NEED ACCESS-KEY:** Contact service provider to get Access-Key

# FRONT-END VIEW:

**in-mac : Machine Generated Bioactivity Platform for Designing Analogs**  
(A Bioassay Guided Tool for Potential Therapeutic Molecules)

**Query Structure Here**



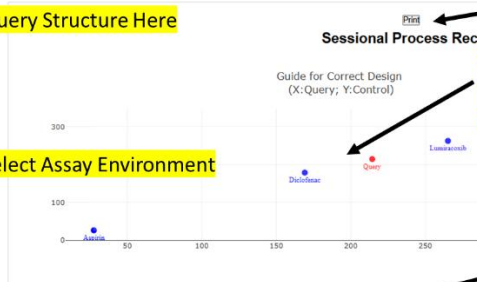
**Select Assay Environment**

Select Assay: COX2  
 MW (approx.): 310.0700 (Limit: 500) / C: 18/ N: 1/ O: 2  
 Running with Pre-Loaded Example Control:  
 Input Control: "Draw it below => Calibrate before use"  
 Query SMILES: O=C(O)Cc1ccccc1Nc2c(Cl)cccc2Cl  
 Control SMILES (after drawing): O=C(O)Cc1ccccc1Nc2c(Cl)cccc2Cl

**Print option**

**Sessional Process Record**

Guide for Correct Design (X:Query; Y:Control)



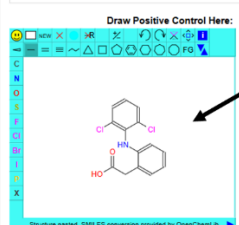
**Area for Dynamic Status of Query In reference of Known active molecules**

**Tabulated Processing Data**

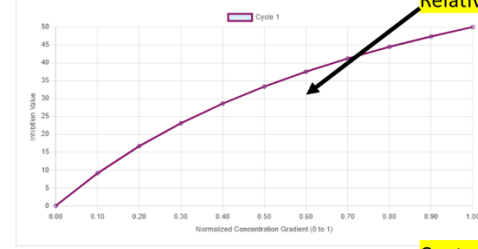
DeleteRow	Assay	Query	Resolution for Assay	In-mac activity (Machine Generated BioActivity)	Control	Inhibition%(alongwith Normalized Conc. Gradient 0-1)	Analog Score	KL_value (Histogram Difference)	Q_Score	C_Score
Delete	COX2	<chem>O=C(O)Cc1ccccc1Nc2c(Cl)cccc2Cl</chem>	0.1596	0.0471	<chem>O=C(O)Cc1ccccc1Nc2c(Cl)cccc2Cl</chem>	0.9,0.9,16.67,23.08,28.57,33.33,37.50,41.18,44.44,47.37,50.00	3.0463	0.000	215.643	215.643

**Reference/Control Structure Here**

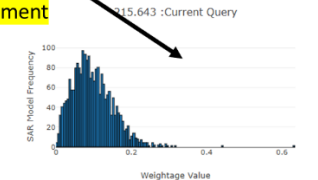


**Relative Inhibition Graph**



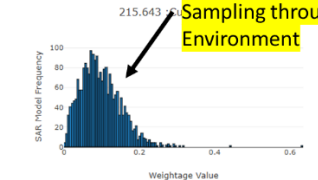
  

**Query Structure Sampling through Assay-Environment**



215.643 :Current Query

**Control Structure Sampling through Assay-Environment**



215.643 :Control

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## VIEW OF EACH CONTENT SEPARATELY:

The screenshot shows a chemical drawing tool with a central canvas displaying a chemical structure of a benzimidazole derivative with two chlorine atoms. A dropdown menu is open, listing various assays. The 'COX2' assay is highlighted in blue. Below the menu, a text box shows the 'Query SMILES' as O=C(O)C1c1cccc1Nc2c(Cl)cccc2Cl and the 'Control SMILES' as O=C(O)C1c1cccc1Nc2c(Cl)cccc2Cl.

1. Step1: Draw the control structure and just confirmed that SMILES has been generated.
2. Step2: Select the Assay Environment.
3. Step3: Draw the query structure and just confirmed that SMILES has been generated.

## EACH INDIVIDUAL CHANGE in QUERY STRUCTURE WILL REFLECT IN GRAPH & TABLE

The screenshot shows the software interface with the chemical structure and the 'Sessional Process Record' graph and table. The graph plots 'Resolution for Assay' (X-axis) against 'In-mac activity (Machine Generated BioActivity)' (Y-axis). The table below the graph provides detailed data for the selected assay and query.

DeleteRow	Assay	Query	Resolution for Assay	In-mac activity (Machine Generated BioActivity)	Control	Inhibition%(alongwith Normalized Conc. Gradient 0-1)	Analog Score	KL_value (Histogram Difference)	Q_Score	C_Score
Delete	COX2	<chem>O=C(O)C1c1cccc1Nc2c(Cl)cccc2Cl</chem>	0.1596	0.0471	<chem>O=C(O)C1c1cccc1Nc2c(Cl)cccc2Cl</chem>	0.9, 0.9, 16.67, 23.88, 28.57, 33.33, 37.50, 41.18, 44.44, 47.37, 50.00	3.0463	0.000	215.643	215.643

## TWO COLUMNS IN TABLE ARE MOST IMPORTANT:

Resolution for Assay	in-mac activity (Machine Generated BioActivity)
0.1596	0.0471

Each individual change in query structure will reflect in graph & table.

1. In-mac activity value is directly proportional to the potency of molecule in context of Assay environment and Positive control provided.
2. Resolution of Assay is representation of in-compatibility of ligand for assay-environment. i.e. Low-resolution value shows high compatibility of ligand for assay-environment, and vice-versa.

## PREPARATION OF ANY EXPERIMENT:

1. Step1: Draw the control structure and just confirmed that SMILES has been generated.
2. Step2: Select the Assay Environment.
3. Step3: Draw the query structure and just confirmed that SMILES has been generated.
4. For generation of data, make changes within the query molecule/ OR change the complete query molecule; and repeat the process.

Each individual change in query structure will reflect in graph & table.

**DELETION OF USELESS ROW FROM TABLE:** each individual row contains delete button; any useless row can be deleted.

**OBSERVATION OF QUERY MOLECULE:** If the query molecule (red-dot) reaches at diagonal of graph, that means Query has similar functional activity as Control molecule in the selected assay environment.

**CREATING REPLICA OF EXPERIMENTS:** Just do 'undo' & 'redo' of query structure, replicas will be generated.

**ANALYSIS OF DATA:** Generate the experiment data and put into excel sheet and do any analysis for it. An online facility has been provided for such data observation/ analysis, here is the link:

'[https://assay.smallmoles.com/cbbeapps/analysis\\_app/analog\\_analysis\\_visual.html](https://assay.smallmoles.com/cbbeapps/analysis_app/analog_analysis_visual.html)'.