Manual

in-mac : Machine Generated Bioactivity Platform for Designing Analogs

(A Bioassay Guided Tool for Potential Therapeutic Molecules)

Index:

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.

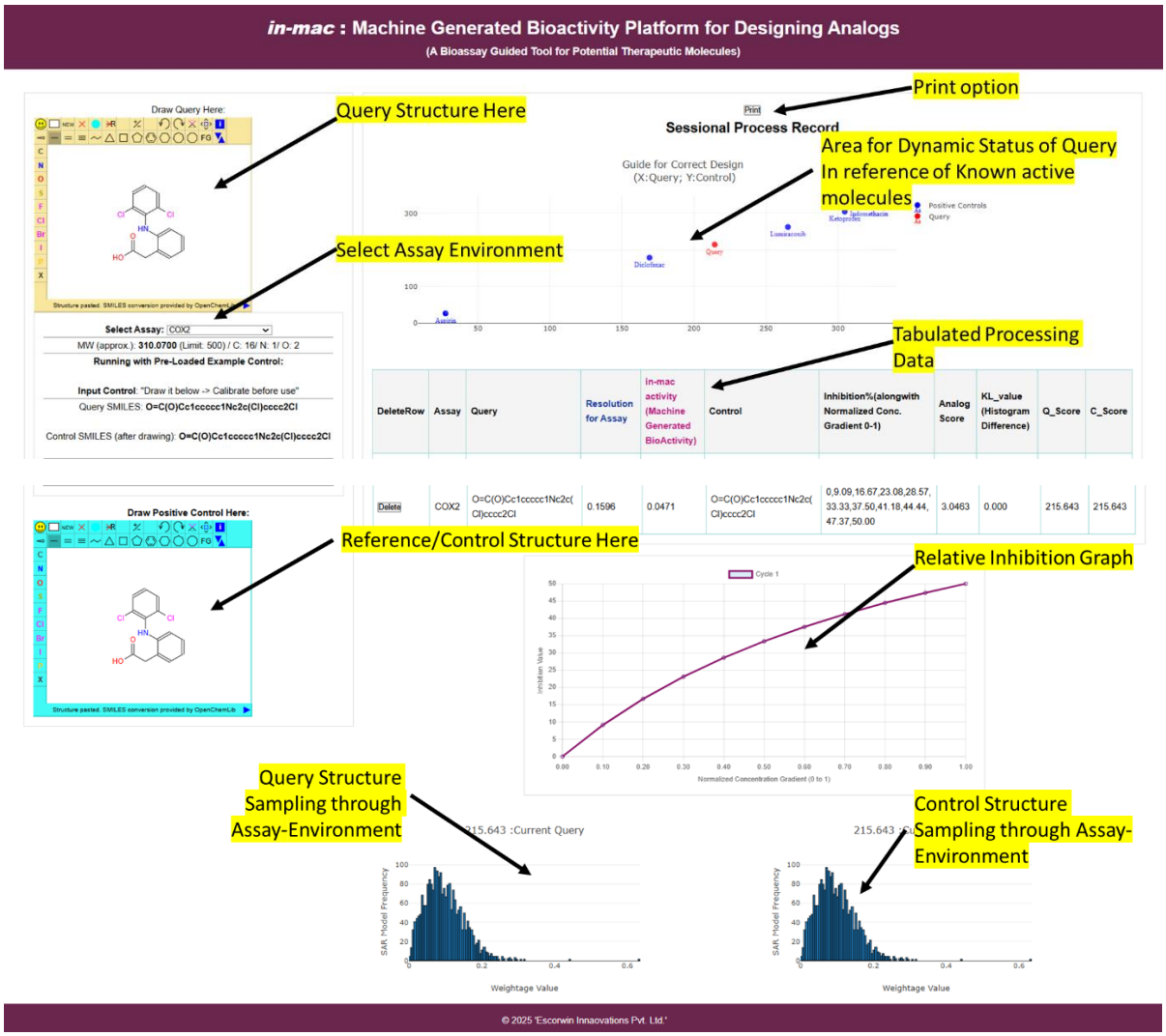
This environment is built using empirical data, and users can select a specific biological target or cell line from a drop-down menu. The *in-mac value* is then calculated based on three key components:

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

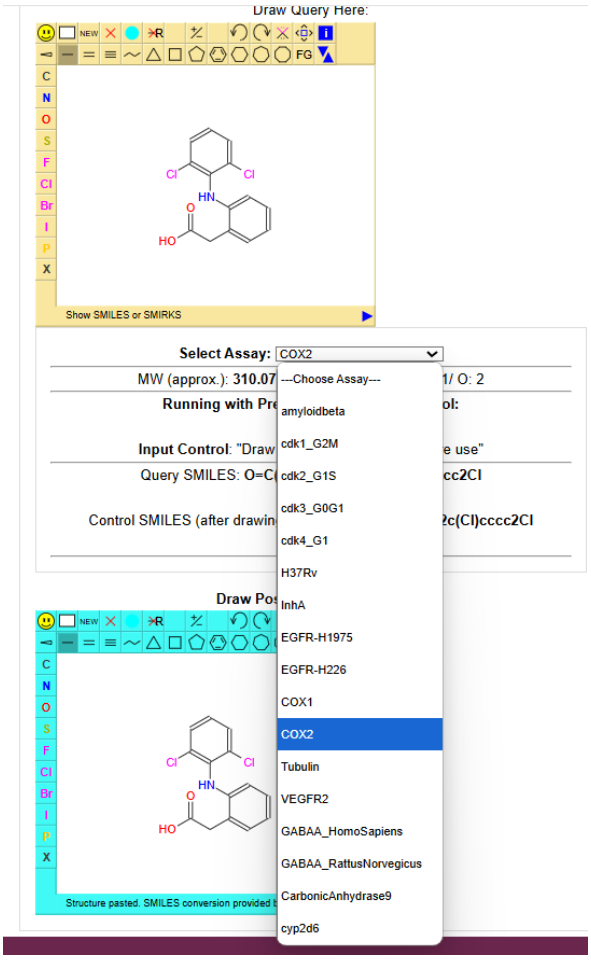
It's important to note that the *in-mac value* is **not** equivalent to in-vitro or in-vivo measurements. Instead, it should be interpreted in the context of the reference/control molecule within the same machine-generated assay environment. This makes *in-mac* a useful tool for guiding the design and 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:

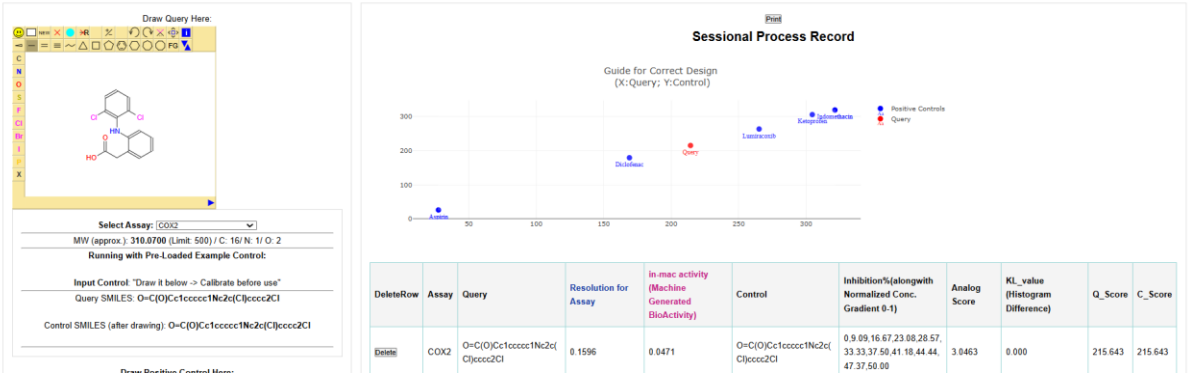


VIEW OF EACH CONTENT SEPARATELY:



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



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'.