Microcare
Laboratory &
Tuberculosis Research Centre

Accelerate Your Synthetic Chemistry research with in Silico Solutions

Are you a synthetic chemist struggling to identify promising drug candidates from your vast compound library? Our in-silico drug discovery services can help you streamline your research and accelerate the discovery of novel compounds with desired properties.

Our Services

QSAR-Based Activity Bioactivity Prediction

- **What it is:** Quantitative Structure-Activity Relationship (QSAR) models correlate the chemical structure of compounds with their biological activity.
- **How it helps:**
  - Predict the biological activity of your compounds before synthesis, saving time and resources.
  - Identify structure-activity relationships to guide your synthetic efforts.
  - Can guide you for optimize compounds for improved potency and selectivity.
- **Applications:** Drug Discovery, Enzyme inhibition, Cancer cell proliferation, and more.

ADME and Toxicity Prediction

- **What it is:** Computational methods to assess the Absorption, Distribution, Metabolism, and Excretion (ADME) and potential toxicity of compounds.
- **How it helps:**
  - Assess the ADME and potential toxicity of your compounds early in the drug discovery process.
  - Help you to design and synthesize safer compounds and reduce the risk of adverse effects.
  - Reduce the likelihood of adverse drug reactions
- **Applications:** Predicting ADME, toxicity, Carcinogenicity, mutagenicity and LD 50

Molecular Docking

- **What it is:** A computational technique to predict the binding mode and affinity of small molecules to protein targets.
- **How it helps:**
  - Predict the binding mode and affinity of your compounds to target proteins.
  - Identify potential drug candidates with high affinity and selectivity.
  - Help you to Optimize lead compounds for improved binding affinity and selectivity
- **Applications:** Virtual screening, ligand optimization, and protein-ligand interaction studies.

MD Simulation

- **What it is:** A computational method to simulate the dynamic behaviour of biomolecular systems.
- **How it helps:**
  - Study the dynamic behavior of your compounds and their interactions with proteins.
  - Gain insights into the mechanism of action of your compounds.
  - Help you to Optimize your compounds for improved efficacy and stability.
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- **Applications:** Ligand Target complex interaction and stability study, enzyme kinetics, and drug discovery.

MICROCARE Laboratory 105, Manthan Point, Una Pani Rd, Lal Darwaja, Haripura, Surat-395003, Gujarat, India
Web : https://www.microcarelab.in, Email: insilicosurat@gmail.com, Phone: 0261-2450049

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Data Submission Guidelines

Required Information:

- **Project Title:** A brief description of your project.
- **Target Protein:** The target protein or enzyme of interest.
- **Desired Activity:** The specific biological activity you want to predict or study.
- **Reference:** Relevant research paper
- **Contact Information:** Your name, email address, and phone number.

Data submission Format:

- Excel containing details of Name of all the compound, Unique code and structure in SMILES (Simplified Molecular Input Line Entry System)

Data Submission: Email: Send your data to **insilicosurat@gmail.com**

Pricing

- **QSAR-Based Activity Bioactivity Prediction:**
  - Ten compounds prediction: [Academic 500, Industry: 1000]
- **ADME and Toxicity Prediction:**
  - Ten compound prediction: [Academic 500, Industry: 1000]
- **Molecular Docking:**
  - Ten compounds docking against one protein: [Academic 1000, Industry: 2000]
- **MD Simulation:**
  - Single-compound MD simulation: [Academic 5000, Industry: 10000]

Note:

- Prices may vary based on project complexity and data size. Please contact us for a customized quote.
- While in silico methods are powerful tools, it's important to note that they rely on computational models based on existing data. For novel chemical structures with unique properties in some cases the accuracy of in silico predictions may be limited.
- Upon submitting your data, our team of experienced scientists will conduct a comprehensive analysis using state-of-the-art computational techniques. We will provide you with a detailed report in soft copy that includes:
  - **Clear and concise results:** Easy-to-understand interpretations of your data.
  - **Detailed methodology:** A step-by-step explanation of the computational methods employed.
  - **Relevant references:** Citations to support methodology.
- **Additional Services:** For more in-depth analysis, customized reports, assistance with data interpretation, Guidance for thesis writing: Expert advice on how to effectively present your results in your thesis. we offer additional services at competitive rates. Please contact us to discuss your specific needs and obtain a detailed quote.
- **Additional Information: [A] Turnaround Time:** depends upon the size and complexity of work **[B] Confidentiality:** We maintain strict confidentiality for all client data **[C] Data Security:** We implement robust security measures to protect your data **[D] Custom Services:** We can tailor our services to meet your specific needs.

Call to Action *Contact us today to discuss your in-silico drug discovery needs. Let's work together to accelerate your drug discovery process. Mail us on* ***insilicosurat@gmail.com for any further details***

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Web : https://www.microcarelab.in, Email: insilicosurat@gmail.com, Phone: 0261-2450049