EU4Health Programme EU4H-2021-PJ2

NEWROAD – GA No: 101080024

*NEWROAD Drug Discovery Platform
User Manual Presentation*

📅 30/10/2023

🗺 N/A

NEWROAD Drug Discovery Platform Introduction

Biovista, WP4

Open Platform for European Networking and Repurposing of Oncological Assets and Drugs

https://new-road.eu/

Introduction to the NEWROAD Visual Explorer

NEWROAD Visual Explorer enables users to:

- access & explore
- create & share networks
- find connections

between analysed elements, based on the scientific literature & structural-related data
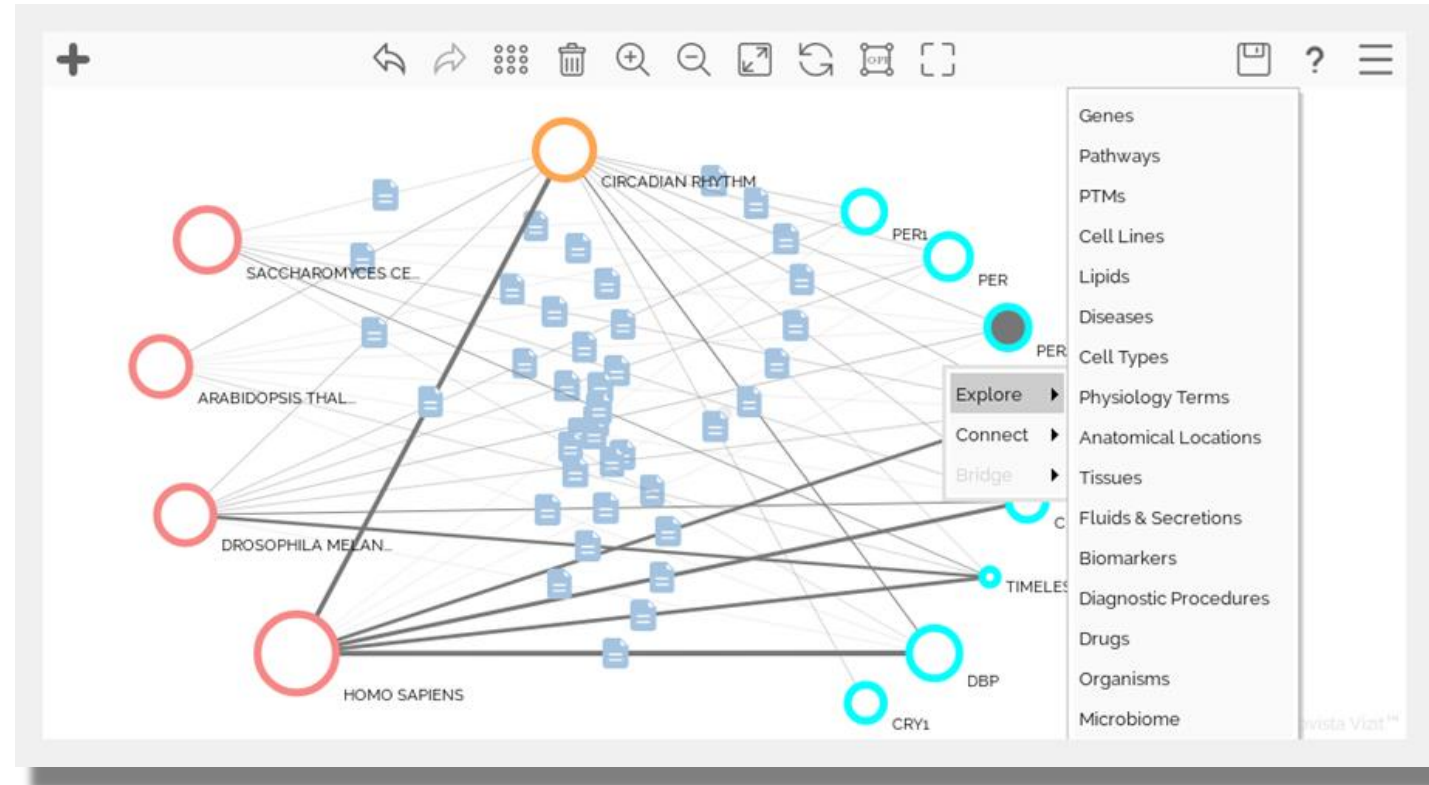
The Literature Search module

The Literature Search module gives scientists and medical professionals a new way of using the literature to advance their work

Literature Search module users

- Type in a search term, instead of a list of publications and get a **visual network** of related terms
- **No longer need to shift through long lists of paper titles** to find the ones they want
- Can **save** the networks they create and **share** their insights with their **peers**

Example of Literature Search module Graph

The Literature Search module

Users can

- search graphs of **relationships** between concepts of interest (e.g. genes, diseases, compounds and cell types)
- obtain an **overview** of the knowledge that is captured in scientific literature (PubMed/MEDLINE)

Drill down to the underlying literature; explore these relationships in depth

Literature Search allows users to search, understand, discover, capture, organize and share knowledge in a single, easy to use environment

Literature Search Supporting Evidence

Molecule and Protein Target Visualization

Exploring Structural Aspects

Molecule and protein visualization within the NEWROAD platform serve as a crucial element for understanding the **structural** aspects of compounds and their **interactions** with biological targets

Protein Interaction Analysis

- **Protein Interaction Networks**: Explore the **networks** of protein-protein interactions related to your research
- **Functional Insights**: Gain insights into the **functional relationships** and **associations** between proteins
- **Data Visualization**: Utilize **charts** and **graphs** to interpret **protein interaction** data effectively
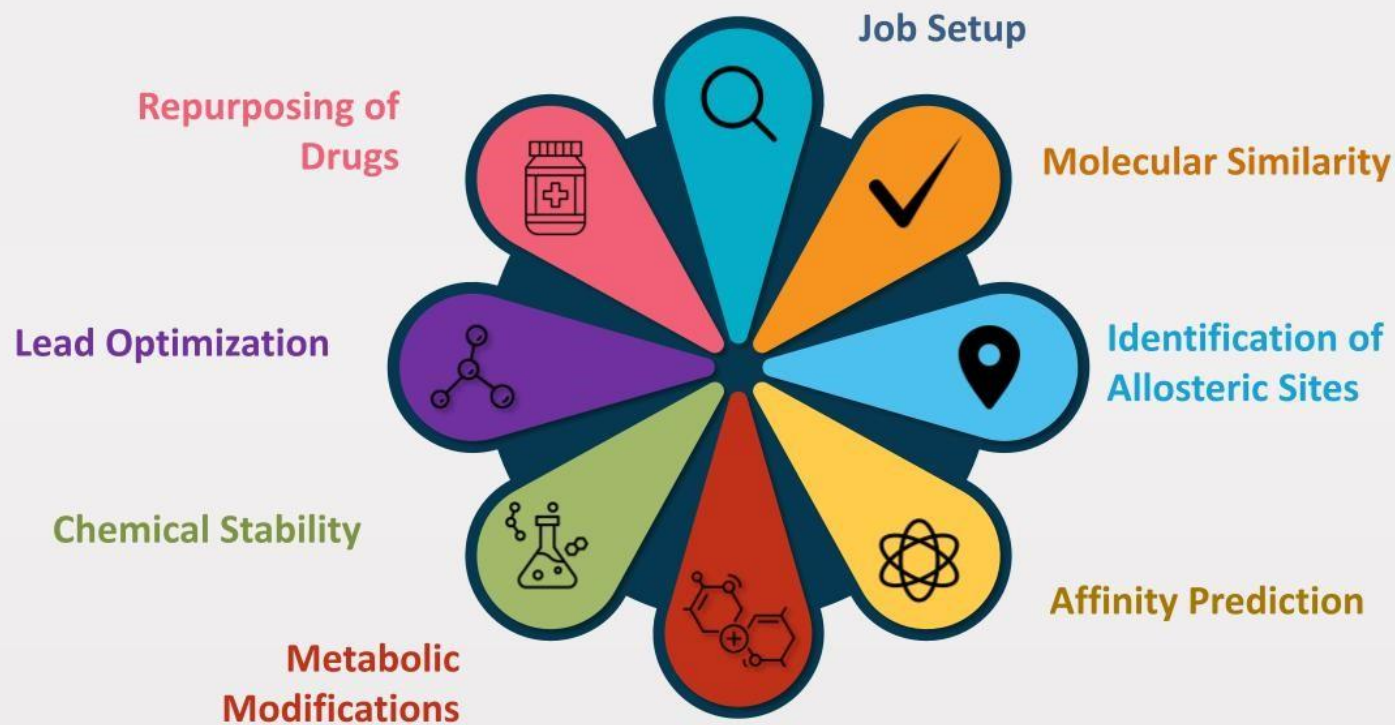
Calculations

Diverse array of calculations for Systematic Drug Repurposing

Calculations encompass various aspects crucial for the **identification**, **evaluation**, and **optimization** of potential drug candidates

Calculations

- **Job Setup:** Module for configuring job parameters, input data, and monitoring progress for various calculations.
- **Molecular Similarity:** Identify molecules similar to a reference compound based on structural characteristics, aiding in the identification of potential repurposing candidates.
- **Identification of Allosteric Sites:** Locate regulatory regions within biological targets to explore new mechanisms of action for existing compounds.
- **Affinity Prediction:** Predict the binding affinity of compounds to target proteins, facilitating the identification of potential repurposing opportunities with high binding affinities.
- **ADMET Properties:** Evaluate the compound's Absorption, Distribution, Metabolism, Excretion, and Toxicity properties to assess its suitability for repurposing.
- **Metabolic Modifications:** Explore how compounds are processed within biological systems, providing insights into their behavior within the body.
- **Chemical Stability:** Assess the stability of compounds to ensure they remain effective in their new context during drug repurposing.
- **Lead Optimization:** Refine and select promising repurposing candidates by analyzing structure-activity relationships.
- **Repurposing of Drugs:** Analyze existing drugs to identify potential candidates for repurposing in the context of oncology.

Semantic Analysis

Semantic analysis in the NEWROAD platform enables the following:

- **Data Interpretation**
  - **interpret** and **understand** data in a more context-aware manner
  - help researchers in identifying subtle **connections** and **patterns** that might not be immediately evident

- **Conceptual Relationships**
  - recognize conceptual **relationships** between genes, diseases, compounds, and other data points
  - deeper **understanding** of the data's **significance**

- **Data Integration**
  - effective integration of disparate data sources.
  - data alignment/common understanding → **easier to correlate information from various domains**

- **Pattern Recognition**
  - recognition of patterns and associations within complex datasets
  - enables researchers **pinpoint potential repurposing candidates and insights**

Automatic Reporting

The NEWROAD platform streamlines the reporting process by <u>automating the creation of reports</u>
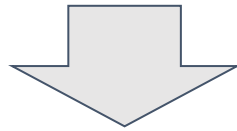
Ensure that researchers can communicate their repurposing candidates and strategies efficiently!

- **Report Generation**: The platform **automatically compiles data** and analysis results into comprehensive reports

- **Customization**: Users can **customize report templates** to include **specific data points** and insights that are most relevant to their research

- **Accessibility**: Generated reports can be easily **accessed** and **shared** with collaborators or stakeholders

Collaborative Login and Space Management

The platform creates an environment for users to **work together**, **share data**, and **collaborate** seamlessly

This feature is designed to enhance user engagement and promote effective teamwork

- **User Authentication:** Users can s**ecurely log in** and access their dedicated spaces within the platform
- **Workspace Creation**: Users have the ability to **create dedicated workspaces** for their organizations based on specific research and collaboration needs
- **User Permissions**: The platform allows for the assignment of **different levels of access** and **permissions** to users within workspaces. This ensures that data and resources are protected while facilitating collaboration
- **Data Sharing**: Users can **share** their work with authorized colleagues, both within and outside their organizations. Sharing can be controlled to ensure **data privacy and security**

Support and Help

Accessing the Knowledge Base

- **Comprehensive Guides**: Access detailed guides, manuals, and tutorials related to platform functionalities, calculations, and data interpretation
- **Frequently Asked Questions (FAQs)**: Browse a collection of frequently asked questions and their answers to address common queries
- **Video Tutorials**: Explore video tutorials that provide step-by-step instructions on using specific features or conducting calculations

Contacting Support

- **Contact Channels**: Users can reach out to support through various contact channels, including email, chat, or a dedicated support portal
- **Issue Resolution**: The support team is available to assist users in resolving technical or platform-related issues
- **User Guidance**: Support can provide guidance on best practices, platform usage, and help address user concerns

NEWROAD

Open Platform for European Networking
and Repurposing of Oncological Assets and Drugs

https://new-road.eu/