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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/>



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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



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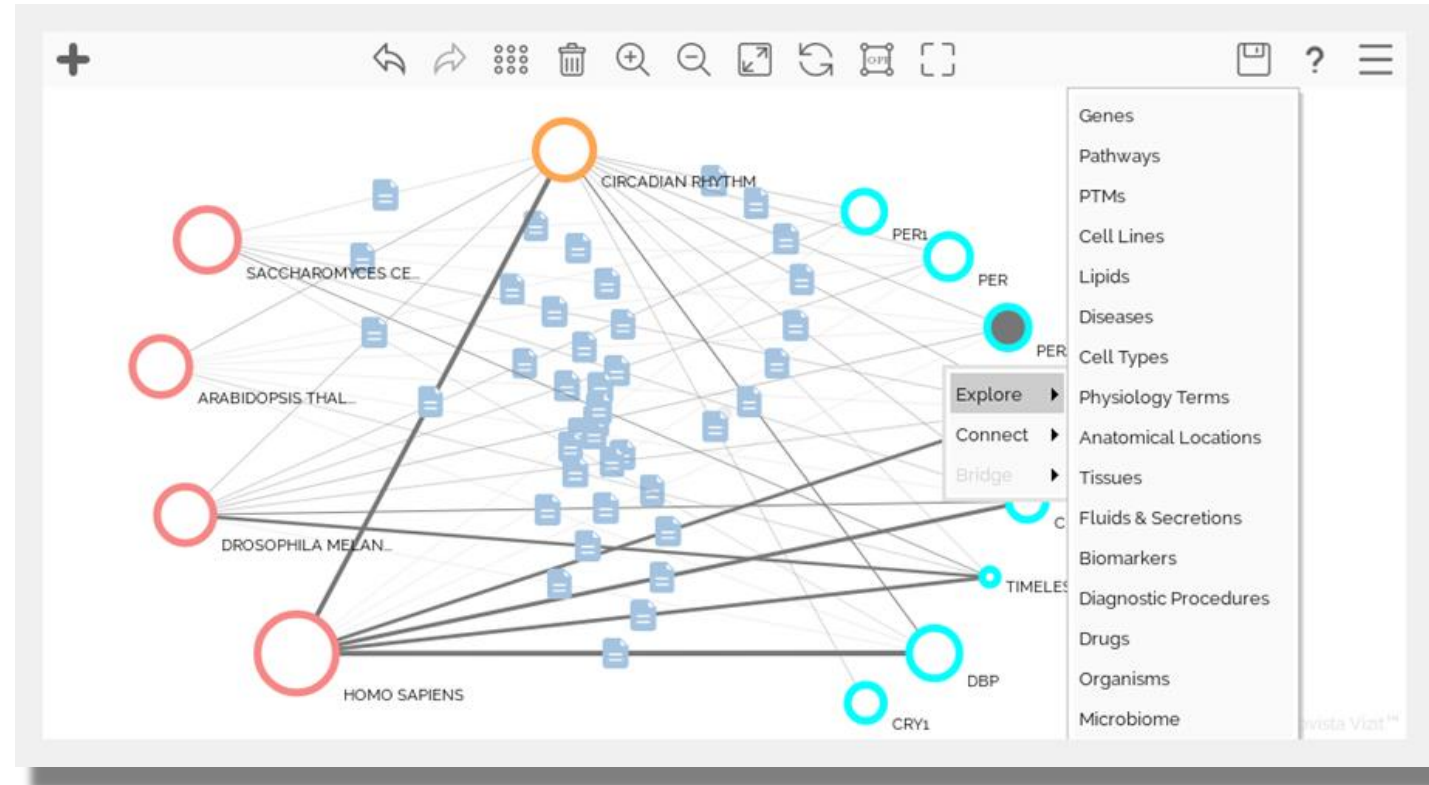
The Literature Search module



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



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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

The screenshot shows a web interface for a literature search module. On the left, there is a network graph with a central orange node labeled "CIRCADIAN RHYTHM (Pathway) - PER1 (Gene)". This central node is connected to four larger red circular nodes on the left, labeled "SACCHAROMYCES CE.", "ARABIDOPSIS THAL.", "DROSOPHILA MELAN.", and "HOMO SAPIENS". Each of these red nodes is further connected to a cluster of smaller blue square nodes. On the right side of the interface, there is a panel titled "CIRCADIAN RHYTHM (Pathway) - PER1 (Gene)". At the top of this panel, it says "Show 10 entries" and has a "New Tab" button. Below this is a "Bibliography" section with five numbered entries, each providing a title, journal name, volume, page numbers, and a PubMed ID. The entries are:

1. 'The effect of high fat diet on daily rhythm of the core clock genes and muscle functional genes in the skeletal muscle of Chinese soft-shelled turtle (Trionyx sinensis).' *Comp Biochem Physiol B Biochem Mol Biol*, Nov, 2017, vol. 213, pp. 17-27, Pubmed: [28729066](#)
2. 'An individual 12-h shift of the light-dark cycle alters the pancreatic and duodenal circadian rhythm and digestive function.' *Acta Biochim Biophys Sin (Shanghai)*, Oct, 2017, vol. 49, pp. 954-961, Pubmed: [28981604](#)
3. 'Hypothalamic control systems show differential gene expression during spontaneous daily torpor and fasting-induced torpor in the Djungarian hamster (Phodopus sungorus).' *PLoS One*, Oct, 2017, vol. 12, pp. e0186299, Pubmed: [29023516](#)
4. 'Macromolecular Assemblies of the Mammalian Circadian Clock.' *Mol Cell*, Sep, 2017, vol. 67, pp. 770-782.e6, Pubmed: [28886335](#)
5. 'Repeated manganese administration produced abnormal expression of circadian clock genes in the hypothalamus and liver of rats.' *Neurotoxicology*, Sep, 2017, vol. 62, pp. 39-45, Pubmed: [28511934](#)

Literature Search Supporting Evidence



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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

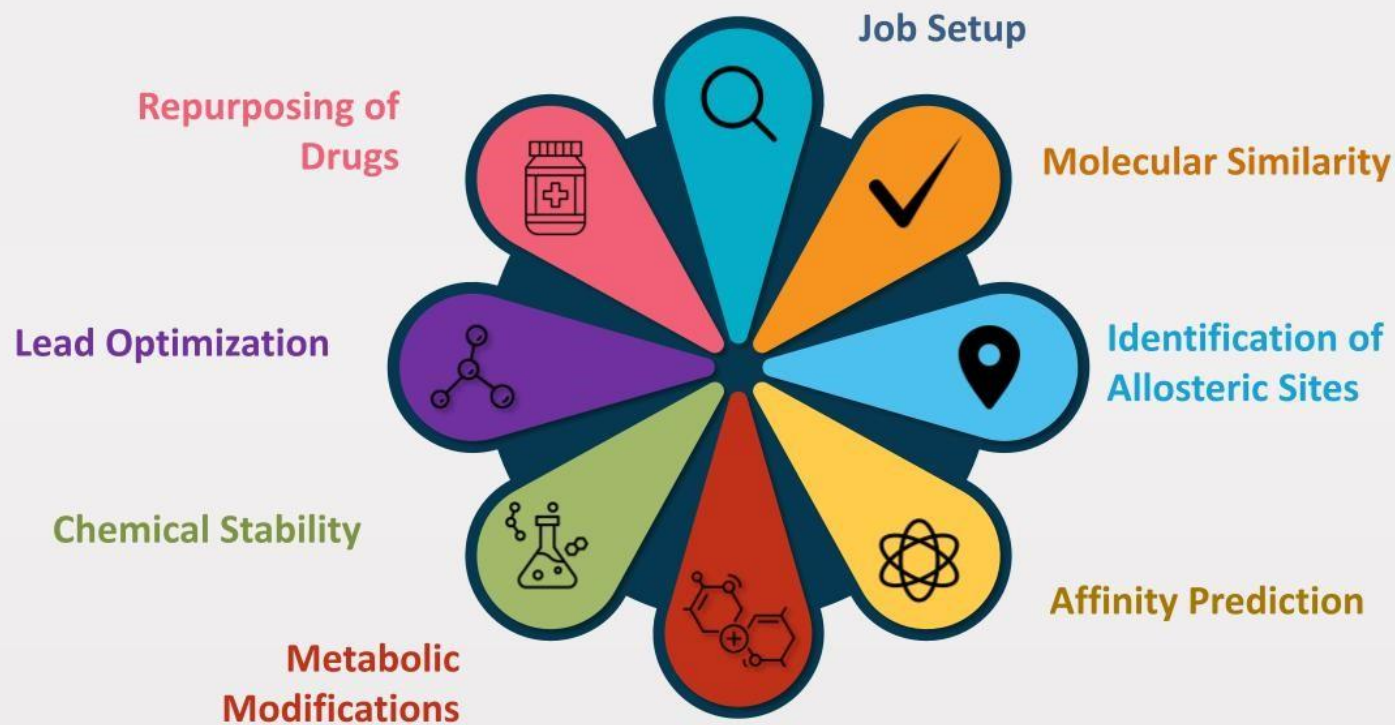


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Diverse array of calculations for Systematic Drug Repurposing

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

Calculations



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.



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Semantic analysis in the NEWROAD platform enables the following:

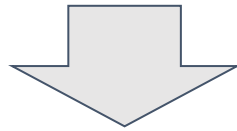
- **Data Interpretation**
 - **interpret** and **understand** data in a more context-aware manner
 - help researchers in identifying subtle **connections** and **patterns** that might not be immediately evident
- **Conceptual Relationships**
 - recognize conceptual **relationships** between genes, diseases, 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 automating the creation of reports



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



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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 **securely 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**.



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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



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