

IPHRONESIS FOR DRUG DISCOVERY & DEVELOPMENT

ABSTRACT

OptraHEALTH™ presents iPhronesis™: The Machine learning based BigData Analytics Platform with Knowledge automation engine for Life science & healthcare markets .

iPhronesis™ is built specifically to address the growing needs of the pharmaceutical industry. Advanced research in drug development is generating novel data at an unprecedented rate than ever before making BigData analysis a challenge. iPhronesis™ makes working with BigData simple by combining pharmacological/ bioinformatics and 'omic' databases with unstructured disparate data integrated into an interactive workflow designer, powerful analytics engine deployed on cloud architecture and using BigData environment with visualization tools for quick, accurate and innovative ways to interpret hypothesis and experiments. iPhronesis™ empowers users to generate insights into complex datasets simply and easily commonly required for drug repositioning and in-silico drug design.

IPHRONESIS™ MODULES

The following is a list of iPhronesis™ modules that are readily available.

DATABASES

iPhronesis™ provides many different databases commonly used in the drug discovery and development processes. Each database undergoes a manual schema curation process wherein we add additional information to help users understand the data better. iPhronesis™ specifically addressed EMR data acquisition as it as being more commonly used for studies in drug toxicity and clinical trials. For unstructured data such as from experimental databases, like GEO, we use machine learning techniques to map schemas and entities. Each mapped entity undergoes manual validation process. Following is a list of few databases which are currently available.

Databases			
Pharmacological & Drug	Proteomic	Genomic	Clinical
SIDER FDALabel DGldb STITCH	BIND MINT PRIDE GelMap	GEO 1000 Genomes dbGAP dbMHC	Ovarian Cancer EMR Systems ClinicalTrials.gov

ChemDB PubChem			
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The following is a list of EMR connectors that are currently available.

EMR Connectors			
EPIC(open.epic.com)	AllScripts(AllScripts Dev)	VistA(Open Source)	Practo

WORKFLOWS

iPhronesis™ provides an interactive, domain specific, template based, workflow module that allows users to quickly and efficiently define workflows which in turn use algorithm to address specific functionality. The workflow editor is implemented in HTML as canvas object and allows for smooth drag drop etc. Nodes represent algorithm, users choose from a wide variety of algorithms depending on the use case, which are supported by customizable parameters.

The following is a list of algorithms available for DDDT applications.

Machine Learning Algorithms		
Categories	Algorithms	
Clustering	Apriori	K-Means/Median
Regression	C4.5 / C5.0	Iterative Dichotomiser 3 (ID3)
Classification	Backpropagation	Hopfield Network
Association	Multinomial Naïve Bayes	Principal Component Analysis
Statistical Classification	Hidden Markov Model	Self-Organizing Map
Probabilistic Model	Support Vector Machine	Bayesian Belief Network
Imaging	Additive Regression	Deep Boltzmann Machine
NLP	Logistic/Linear Regression	Deep Belief Networks
		Linear Discriminant Analysis
Pipelines		
Ruffus	Cloud Scaler	HDFS
Luigi		
Domain Focus		
Drug Repurposing and toxicity	Molecular Interactions	Cohort Designer
Drug-Drug Interactions	Novel Insights	Smart Clinical Trial Designer
		Disease Analysis and Predictor

VISUALIZATIONS

iPhronesis™ provides a suite of visualization widgets that make viewing complex datasets simple. The selection of a visualization widget is determined when the workflow is designed but may be optionally

changed when viewing the data. iPhronesis™ intelligently detects if a certain data view is allowed for a certain widget and only shows compatible widgets for user to view.

The following visualization widgets are currently available.

Visualization		
<i>Core DDT Analytics</i>	<i>Others</i>	
Box Plots Outliers Tree Maps Sunburst Tree Layout Timelines Sanky Bar charts Line charts Bubble Charts Dendrogram Force layout Stream tracing Bivariate Area Chart	Data tables with sort, order and tag functionality Segmental and normalization plots Variation viewer	Concept diagrams HeatMaps Cluster Maps Network diagrams

All visualization widget uses the latest charting libraries and several are custom built. This approach allows for viewing data in a very precise manner and client side rendering takes the user experience to the next level.

INTERPRETATIONS

A workflow is only complete when it delivers powerful interpretations. iPhronesis™ provides industry standard workflows specifically for the pharmaceutical industry to get you quickly up to speed and instantly start using validated, approved and performance tuned workflows leading to high interpretative power. In drug discovery and development applications such workflows are typically used for in silico drug design, to gauge drug efficacy and toxicity and for drug repurposing studies. Users interpret the data using the built-in analytics power of iPhronesis™ that allows for visualizing data in novel ways. An example is viewing drugs, side-effects and patients all in one concept plot. Drill down capabilities allows for changing the view dynamically and view evidences for each entity on the chart. Another example is to generate a list of up and down regulated genes when cells are treated by a certain anti-malignant agent. iPhronesis™ then generates a network graph of connected genes and recursively its side effects and regulation patterns. There are many use cases.

Following is a list of ready-to-go domain workflows available in iPhronesis™.

<i>DDDT Workflows</i>	<i>Others</i>
In- silico drug discovery Cohort Design Drug Repurposing Drug Efficacy & Toxicity Drug Signatures Disease Signatures	Insights Based on NLP Drug- gene interactions Correlation of experimental findings with EMR records.

KNOWLEDGE AUTOMATION

The process of interpretations is only complete when concrete scientific evidences are provided. At times such data is buried un structured data and is not semantically organized. iPhronesis™ bridges this gap by providing a very powerful module that ingests data from scientific literature and contextually connects literature with interpretations such as drug- gene interactions, drug signatures or structural activity of drugs. This allows for rapidly identifying targets of drugs of interest, identifying false positives, ascertaining efficacy and potency in comorbid conditions etc. Such evidence based insights are available in iPhronesis™, additionally, there is also a BioNLP (Bio Natural Language Processing) interface that allows users to compose queries in natural language, parsing which iPhronesis™ provides results.

For more information and demo please contact us today on info@optrahealth.com
