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# Product Overview Document

## Discovery Central Version 1.0

### 1] Introduction

#### What is Discovery Central?

Discovery Central Version 1.0 is an enterprise software solution for the pharmaceutical and bio-informatics industry to facilitate Drug Discovery.

Facilitating the processes, procedures and policies that most suit those involved in drug discovery endeavors, this product leverages and automates processes typically performed in a drug research and development organization.



*Discovery Central : Promises to transform the way one works!*

#### Intended Community:

People who are in the drug discovery process are the intended audience.

From the person who sets the experiment protocols in place, to the one who dispenses the compounds to the one who conducts the experiments and enters in the parameters of the results, are all the intended recipients of the application's functionality and usage.

#### Rationale for the application:

Some of the genuine needs, problems, requirements of a drug discovery software solution and how Discovery Central addresses them as inherent functions of its structure and implementation are listed below:

- **Drug Discovery Process Management :**

A system that is coordinated, automated and dependable is required.

At the core of Discovery Central's architecture is a Java-based Business Process Manager (BPM) which automates the processes that are specified in the user created drug discovery related workflows.

The BPM monitors the experiments in each of the workflow steps, their rules and constraints and appropriately generates tasks and dispensary requests and takes other workflow step progression measures.

The coordination between personnel, policies and procedures is aptly managed at an enterprise level by the BPM.

- **Drug Discovery Data Management :**

Coordinated and secure data management and porting of data is needed.

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Experimental and process data is securely collected and stored for further analysis, processing and monitored access.

Moreover Discovery Central is a coordinated system and centralized as it is server based and hence provides the appropriate personnel with the latest sample and process information and maximizes information flow across the various departments.

- **Scalable and Extensible Application :**

The application has been built to scale to an enterprise level. The application is extensible as new functionalities can be integrated into it as requirements emerge.

- **Drug Discovery Context :**

A system is required, but one that speaks the same language as its users and one which provides the environment and the feel of the drug discovery process.

This application easily adapts and integrates with the personnel's drug discovery activities.

Flexible task assignment and reassignment is made possible.

The solution seamlessly integrates with the day to day working of the personnel and synchronizes their efforts and thus leverages the processes involved in drug discovery.

- **An alternative :**

An alternative is required to the ubiquitous paper-based systems in the drug discovery circles.

Discovery Central efficiently substitutes and at times effortlessly integrates with paper-based systems.

The application eliminates the fallacies that are inherent with paper based data entry forms.

It presents itself as a secure automated system, protects from data loss and reduces data entry and interpretation errors with its inherent validation and verification procedures.

- **Customization :**

Customization is a trait that is expected to be inherently present in a system that is used in the drug discovery process.

Discovery Central has been built on a consultative approach and it possesses the attribute of customization implicitly and further system wide adaptations can be efficiently incorporated.

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## 2] The repertoire of salient functionalities:

- **User Experience:**  
User role orientation and data security are maintained throughout the application.  
  
Users, based on the appropriate roles, are allowed access to certain domains of the system and the information within them. This ensures domain security.
- **Organizational Structure and Setup:**  
The implementation of a hierarchy, based on organization - sections, groups and projects, encourages a corporate setup to the drug discovery division in the organization that uses the product.
- **Project Setup :**  
Appropriate projects can be created to enable concentrated drug discovery processes.
- **Cascades :**  
These are workflows in action. Helps create and manage the entire life spans of cascades and experiments. Users can log in their samples, assign cascades to the samples and record the sample results in the system.
- **Tasks and their management :**  
Coordinated task management is provided.
- **Team Management :**  
Flexible personnel coordination and task assignment is made possible.
- **Managing Samples in the Dispensary :**  
Sample profile management and tracking is easier and centralized.
- **Reports Generation :**  
Laboratory Sample Tracking is made easy. Experiments, as part of the cascades, on samples and their results can be monitored easily.
- **Document Management :**  
Lesser dependency on paper based systems is ensured.

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- **USER EXPERIENCE:**

Discovery Central offers to its users four basic views.

Depending upon the role of the employee who has logged in, each view provides different features and functionalities.



**User Views :** *User View is dependent on the user role.*

**Domain :** *Project Central*

**User Role :** *Project Manager or Group Manager*

**Domain :** *Section Central*

**User Role :** *Section*

For users coming under both of the above domains the following is made available : creation of projects, design and execution of cascades, access to reporting features -project reports and organization reports, management of samples in the dispensary, document management, task management and redirection and team management.

**Domain :** *Task Central*

**User Role :** *Default User*

These users can create projects, handle project reports, manage samples in the dispensary, manage tasks and documents and view cascades.

**Domain :** *Admin Central*

**User Role :** *System Administrator*

A System Administrator manages experiment lookups and subsequent maintenance on experiments, setup of the organization hierarchy, creation and maintenance of projects and loading of lab images of locations of samples into Discovery Central.

- **ORGANIZATIONAL STRUCTURE AND SETUP:**

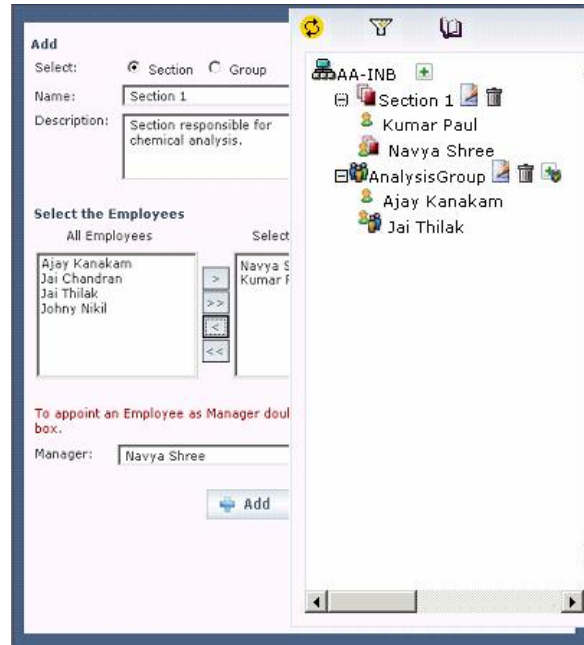
Discovery Central facilitates processes within an Organization. The Organization can have multiple Sections also called as Departments. Each Employee belongs to one Section and each Section has one Section Manager.

Within the Organization, Groups are formed for specific functions. Each Group has a Group Manager and could have one or more Employees in that Group. A Group could contain one or more Groups under it. Each of these Groups would also contain a Group Manager and one or more Employees.

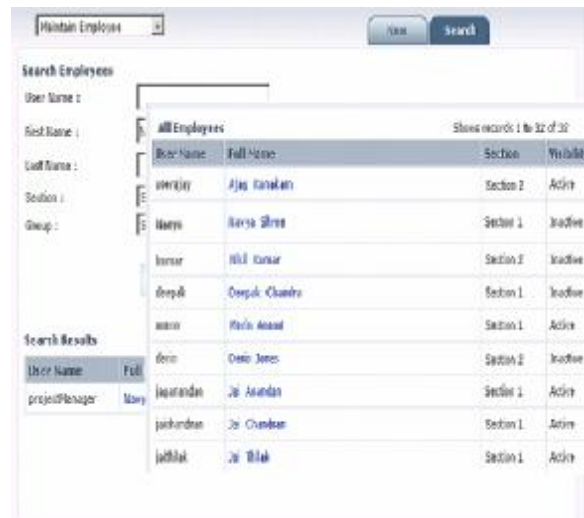
The Organization could also have many Projects. Projects could belong to a Group, Section or exist independent of a Group or a Section. A Project will have a Project Manager and one or more of the Employees. An employee will always belong to only one Section, but could belong to any number of Groups and Project Teams.

**The Setup:**

The System Administrator creates and maintains the Organization, its Sections, Groups, Sub Groups, and Employees. The appointment of managers to the sections, groups, sub groups and projects is done in here. The visibility of groups or sections throughout the application and employee activation and inactivation can be controlled from in here.



**Organization Setup :** Create the organizational structure to best suit one's requirements.



**Maintain Employees :** Create, search and maintain employees efficiently.

- **PROJECT SETUP:**

Projects can be created and maintained within an organization and employees can be assigned as project members. A System Administrator can create and maintain projects, their members and their managers and also manage a project's visibility throughout the application; other users being allowed the privilege to only create projects, their members and their managers.

- **CASCADES : WORKFLOWS IN ACTION**

Since Discovery Central is primarily concerned with facilitating drug discovery, all cascades comprise of a series of experiments, within a series of cascade steps, which need to be performed with one or more chemical compounds.

Managers can design and execute cascades.

Rules are set to logically assess the values of the various constituent variable properties of a given cascade step.

When all the constituent factors of a rule satisfy their threshold constraints, then the rule becomes active.

Appropriate triggers are enabled, based on this logical assessment, to become active when a cascade step reaches a particular status based on the outcome of its constituent experiments. New, In Progress, Delayed and Completed are the four step statuses available.

The trigger is, at times, used to make an auto transition to another cascade step of the many that may follow after a given step.

Initiation of another cascade is also made along the same lines and a listed employee can also be intimated about a cascade step event via email.

Save Cascade

Cascade Name : cascadeOrion

Description : This cascade com experiments relate chemical analysis

Effective Date : 03/03/2006

Expiry Date : 04/08/2007

Save Cancel

Define Step

- Add Experiment
- View All Experiment
- Add Rule
- Add Event Trigger
- View Event Triggers
- Delete

Java Applet Window

**Create Cascades :** Design cascades through the user interface.

Add Experiment

Add Experiment Variable Property

Experiment name : Exp Lt Name

Responsibility : Group

Group : AnalysisGroup

Resource : Ajay Kanakarr

Due in : 24

Priority : Urgent

Add variable property

Property name : varProp1

Data type : Number

Description : This variable property holds the numerical value of the first contro parameter.

Mandatory : Yes

Ok Cancel

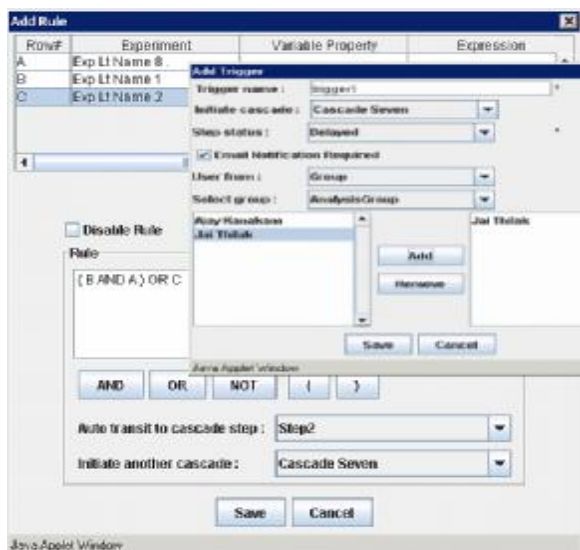
Save Save and Close Cancel

Java Applet Window

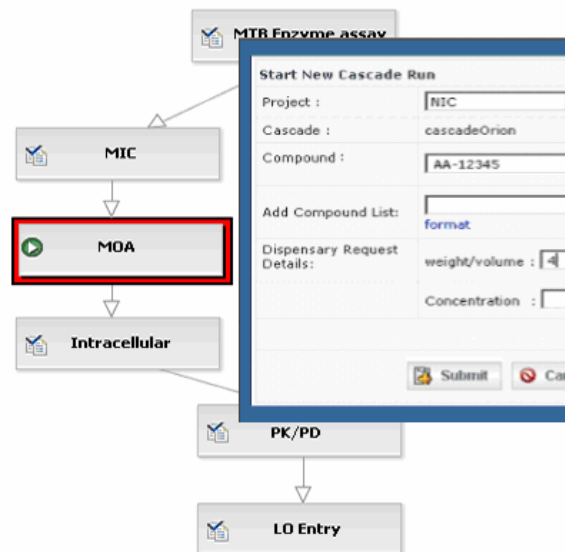
**Setup Experiments :** Set the experiments and the corresponding variable properties.

In addition to generating a task for the resource specified in the cascade step, the dispensing cascade, a predefined cascade that handles all dispensing requests, will be called with Tasks or Requests to dispense the complete set of compounds required for this experiment.

This involves the submitting of both Single Sample Request and Multiple Sample Requests to the compound dispensing authority.



**Rules and Triggers :** Set logical parameters and the course of events.



**Cascades Execution :** Set the required parameters and set the workflow into action.

- **TASKS AND THEIR MANAGEMENT:**

Tasks are primarily auto-generated by cascades for each cascade step. When needed, tasks can also be created by any user and these could exist independently as a one off activity to be performed.

Only tasks which have not reached the completion status and those which are not user generated get higher priority throughout the application.

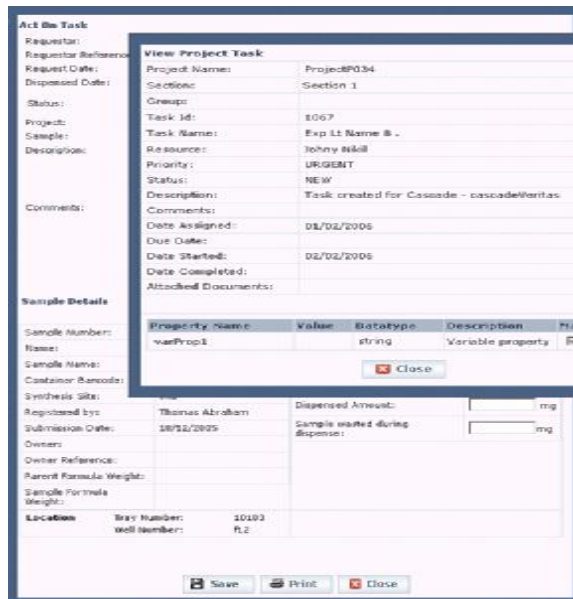
Action Item tasks and the Dispensary Request tasks are essentially the two available types.

The Action Item tasks are those which require an experiment to be performed.

Dispensary Request tasks are handled by personnel in-charge of dispensing the compounds for the experiments.

**Managing tasks via tasklists:**

Tasklists, defined by the user, can be used to group tasks for easier and selective task management.



**Tasks :** Action and Dispensary Requests are the two types available.

### **Communication of miscellaneous tasks:**

Random tasks are user created and are used to assign tasks, including miscellaneous errands, to oneself or to the other employees within Discovery Central. A random task exists independently and can be used to post reminder notes to oneself about ad hoc tasks that one needs to do.

### **Task Redirection:**

Appropriate task redirection is efficiently enabled between employees of the same section or project.

- **TEAM MANAGEMENT:**

Managers can manage the employee task teams within Discovery Central. A brief performance overview of an employee can be obtained in here . This module helps specify all the tasks, and their current statuses, coming under the purview of a listed employee.

The absence of an employee for a particular period can be taken care of by assigning a substitute employee for the same period. This helps make sure that the non availability of an employee during a given period does not affect the execution of a task assigned to that employee. Another available employee within the same section can be re-assigned the task.

- **MANAGING SAMPLES IN THE DISPENSARY:**

Samples can be searched out and their details obtained easily.

Sample names, as part of the search criterion, can also be entered through files.

Requests for samples, from sample lists obtained as part of search results, can be made by the user, depending on the user's profile, through the application.

And as part of their maintenance tasks, managers can setup container and location details of the samples.

Newly registered samples that have just entered the Discovery Central domain from the Oracle queues of an external data source can be viewed and accessed. Location details of the sample including the sample location images and sample details in the form of a report listing can be accessed in here.

Sample Number	Name	Synthesis Site	Status
AA1234567	AA1234567	AA1234567	AA1234567
AA1234568	AA1234568	AA1234568	AA1234568
AA1234569	AA1234569	AA1234569	AA1234569
AA1234570	AA1234570	AA1234570	AA1234570
AA1234571	AA1234571	AA1234571	AA1234571
AA1234572	AA1234572	AA1234572	AA1234572
AA1234573	AA1234573	AA1234573	AA1234573
AA1234574	AA1234574	AA1234574	AA1234574
AA1234575	AA1234575	AA1234575	AA1234575
AA1234576	AA1234576	AA1234576	AA1234576
AA1234577	AA1234577	AA1234577	AA1234577
AA1234578	AA1234578	AA1234578	AA1234578
AA1234579	AA1234579	AA1234579	AA1234579
AA1234580	AA1234580	AA1234580	AA1234580

Sample Search : View sample availability details.

**View Sample**

**Sample Details**

Sample Name:	AA1234567	Owner:	Prahlad, Dwarakanath (kqhp808)
Container Barcode:	12143855	Owner Reference:	MNH-445-121-4
Synthesis Site:	10B	Molecular Weight:	
Registered by:	Mallya, Meenakshi (kqsn418)	Sample Molecular Weight:	
Submission Date:	06/05/2005	Tare Weight:	0.0 mg
		Total Weight:	5.3 mg
		Sample Weight:	5.3 mg

**Location**

Tray id: [ ]  
Well Number: [ ]

Print Close

Container Location

Save Save & Generate Report Cancel

Sample Details : View and Act on samples.

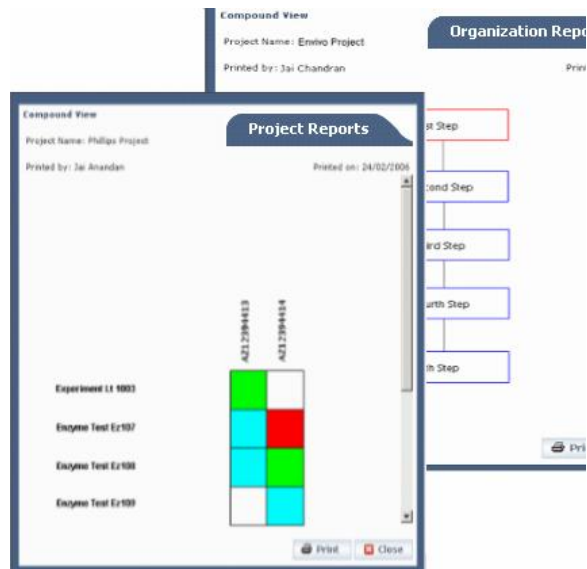
- **REPORTS GENERATION:**  
The application provides essentially two kinds of reports:

**Project Reports:**

Project reports help the user to graphically view sample oriented cascade flows and cascade step statuses of samples for the user related projects.

**Organization Reports:**

These reports help the user to graphically view user related sample cascade flows.



Reports : Graphical reports at the click of a mouse to enhance user experience.

- **DOCUMENT MANAGEMENT:**

Efficient document management under the purview of sections, groups, projects or folders is possible within Discovery Central. The internal document storage functionality encourages lesser paper work.

Context specific documentation, specifications, experiment protocols, notes and explanatory documents can be maintained within and across the different segments of the organization.

### 3] A Customizable Solution :

Discovery Central 1.0 is a fully customizable solution. Additional features and functionality can be added to Discovery Central 1.0.

For more information please contact us:

**New Creation Information Technologies (P) Ltd.**  
 #75, 1<sup>st</sup> Floor, 14<sup>th</sup> Cross, R.T. Nagar, 1<sup>st</sup> Block  
 Bangalore 560 032, INDIA  
[www.newcreationit.com](http://www.newcreationit.com)  
 Email: [business@newcreationit.com](mailto:business@newcreationit.com)  
 Phone: +91-80-23544328 / 329