Kanban in Drug Discovery

Optimizing both drugs and team efficiency

How to optimize team efficiency in a medicinal chemistry project?

Drug discovery is a multi-dimensional mission, in addition to optimizing the molecules, the project leader also needs to prioritize all ongoing activities in the team, such as compound design and synthesis, as well as assay data requests, and results of analysis.

Due to the nature of research there are many uncertainties, making the distribution of work within a team sometimes unbalanced. For instance, it is difficult to estimate the time it takes to synthesize a novel compound or how long until a certain starting material arrives from another country.

Interactive Kanban board for drug discovery

A multi-dimensional, searchable, and interactive Kanban board can help the project team to get a comprehensive overview of the ongoing activities. This facilitates distribution and prioritization of work (Figure 1).

There are also more ambiguous parameters that are equally important for efficiency, such as the estimated time to finalize a task and the estimated cost and value of getting a task done. Visualizing this information via the Kanban board supports decision making (Figure 2, 3 and 4 on page 2).

Kanban is Japanese for 'billboard' or 'signboard' and was first used in the 1950's by car manufacturer Toyota, aiming to improve efficacy and quality of production.

By visualizing both results and rate-limiting factors of the overall process, resources can be shifted from less crucial or problematic tasks, to activities with higher impact.

Also, the transparency of the Kanban board enhances the employees' sense of shared responsibility and enables understanding of issues, thus facilitating innovation.

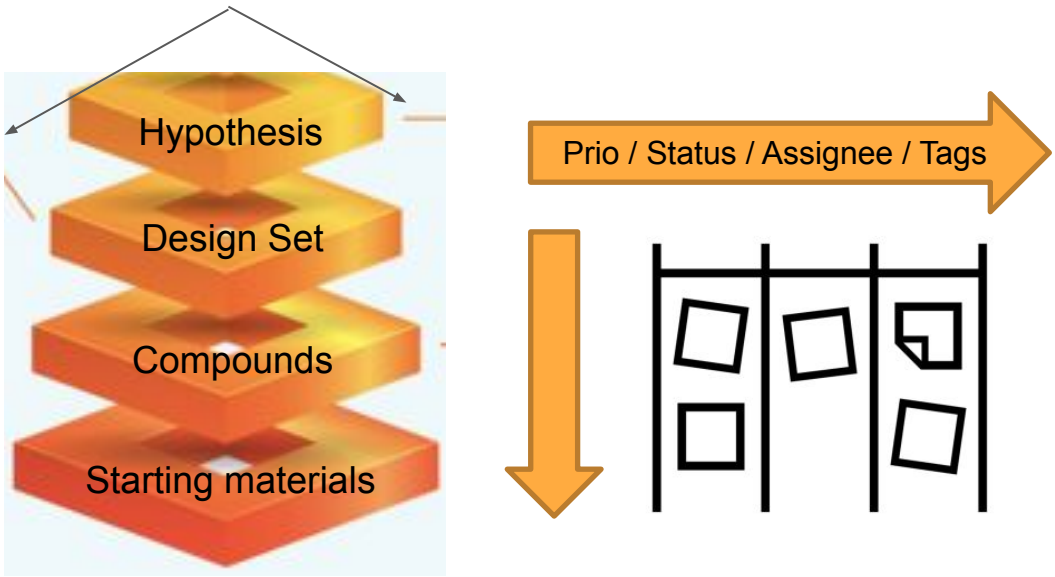

Figure 1. *An interactive Kanban board allows teams to keep track of who is performing which tasks on several levels (Hypotheses, Design sets, and Compounds). Each level can be viewed on a two-dimensional, dynamic board showing assignee, status, priority or tags on any of the axis. Each level is searchable and can be filtered on both text and chemistry. Time spent on each task is automatically measured. Cost and value for each task can be annotated.*

Capabilities of the Design Hub Kanban board

Show, sort, filter on and edit…

- Author
- Assignee
- Chemical structure
- Project
- Status
- Priority
- Tags
- Time spent
- Hypothesis, Design set and Compound hierarchy

Estimating value and time to perform a task

A “task” in drug discovery may be a compound to be synthesized, a predictive model to be developed, or assay data to be generated.

The time to finalize a task can me measured by counting the number of days until a compound has been synthesized (Figure 2). Cost of synthesis can be estimated as well (Figure 3). Visualizing predictions and data for each compound via the Kanban board supports decision making (Figure 4).

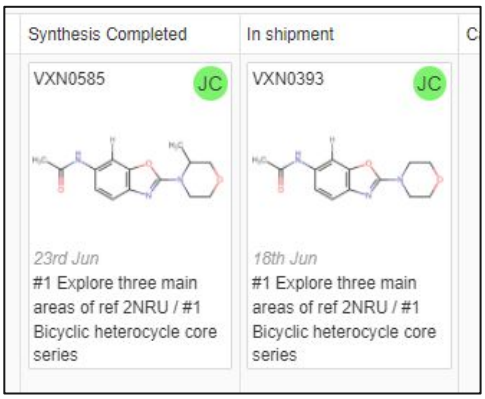

Figure 2. The time spent to finalize each task is automatically calculated, from the point of initializing the task.

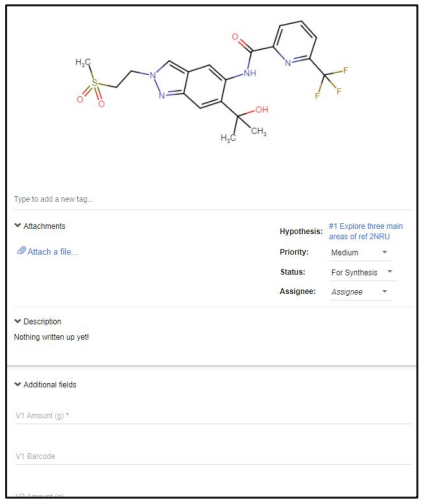

Figure 3. Information on number of synthetic steps to produce a compound, starting material availability and cost can be stored on compound level or accessed via a link into your ELN.

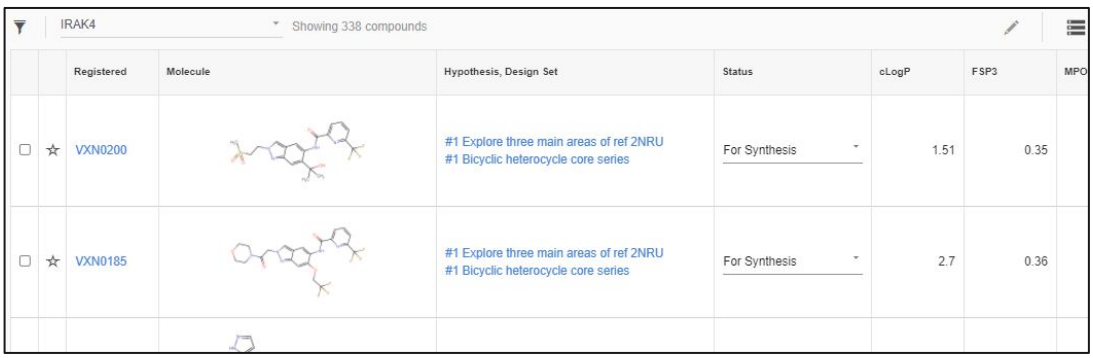

Figure 4. The value of each generated task is reflected by the priority of the task. To decide the value of a certain compound, likely an extensive SAR-analysis has been made, and/or predictive models have suggested how promising this compound is. The Kanban board has direct connections from the planned compound to their corresponding hypothesis, predictions and data.